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(71) JAPAN SCIENCE AND TECHNOLOGY AGENCY,
4-1-8, Honcho
Kawaguchi-shi
332-0012, SAITAMA, XX (JP).
OSAKA BIOSCIENCE INSTITUTE,
2-4, Furuedai 6-chome
Suita-shi
565-0874, OSAKA, XX (JP).
RIKEN,
2-1 Hirosawa
Wako-shi
351-0198, SAITAMA, XX (JP).

(72)

URADE, YOSHIHIRO (JP).
KUMASAKA, TAKASHI (JP).
HAYAISHI, OSAMU (JP).
MIYANO, MASASHI (JP).
KINUGASA, SHIGEHIO (JP).
MATSUMURA, HIROYOSHI (JP).
YAMAMOTO, MASAKI (JP).
IRIKURA, DAISUKE (JP).
INOUE, TSUYOSHI (JP).
KAI, YASUSHI (JP).
OKANO, YOUSUKE (JP).

(74)

KIRBY EADES GALE BAKER

(54) STRUCTURE TRIDIMENSIONNELLE DE PROSTAGLANDINE SYNTHASE D ET SONT UTILISATION
(54) THREE-DIMENSIONAL STRUCTURE OF PROSTAGLANDIN D SYNTHASE AND UTILIZATION THEREOF

(57)

It is intended to provide a method of designing an antiallergic agent, a sleep controlling agent, an antiobestic and a remedy for brain injury acting via the inhibition of the biosynthesis of prostaglandin D2. Crystals of a complex of human-origin hematopoietic prostaglandin D synthase, glutathione and a substrate analog or an inhibitor, etc. are prepared and the three-dimensional structural coordinate of each atom in the complex is determined by X-ray crystal analysis.



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(71) Demandeurs/Applicants:

JAPAN SCIENCE AND TECHNOLOGY AGENCY, JP;
OSAKA BIOSCIENCE INSTITUTE, JP;
RIKEN, JP

(72) Inventeurs/Inventors:

URADE, YOSHIHIRO, JP;
HAYAISHI, OSAMU, JP;
INOUE, TSUYOSHI, JP;
KAI, YASUSHI, JP;

...

(74) Agent: KIRBY EADES GALE BAKER

(54) Titre : STRUCTURE TRIDIMENSIONNELLE DE PROSTAGLANDINE SYNTHASE D ET SONT UTILISATION

(54) Title: THREE-DIMENSIONAL STRUCTURE OF PROSTAGLANDIN D SYNTHASE AND UTILIZATION THEREOF

(57) Abrégé/Abstract:

It is intended to provide a method of designing an antiallergic agent, a sleep controlling agent, an antiobestic and a remedy for brain injury acting via the inhibition of the biosynthesis of prostaglandin D₂. Crystals of a complex of human-origin hematopoietic prostaglandin D synthase, glutathione and a substrate analog or an inhibitor, etc. are prepared and the three-dimensional structural coordinate of each atom in the complex is determined by X-ray crystal analysis.

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(72) Inventeurs(suite)/Inventors(continued): OKANO, YOUSUKE, JP; KINUGASA, SHIGEHIRO, JP;
MATSUMURA, HIROYOSHI, JP; IRIKURA, DAISUKE, JP; YAMAMOTO, MASAKI, JP; KUMASAKA, TAKASHI, JP;
MIYANO, MASASHI, JP

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ABSTRACT OF THE DISCLOSURE

It is intended to provide a method of designing an
5 anti-allergic agent, sleep controlling agent, anti-obestic
agent and remedy for brain injury acting via the inhibition
of biosynthesis of prostaglandin D₂. Crystal of a complex
of human origin hematopoietic prostaglandin D synthase,
glutathione, and a substrate analog or an inhibitor, etc
10 are prepared and the three-dimensional structural
coordinate of each atom in the complex is determined by X-
ray crystal analysis.

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SPECIFICATION

THREE-DIMENSIONAL STRUCTURE OF PROSTAGLANDIN D SYNTHASE AND
5 UTILIZATION THEREOF

BACKGROUND OF THE INVENTION

The present invention relates to three-dimensional structures of hematopoietic prostaglandin D synthase (which
10 may refer to as "PGDS" hereinafter), and a method for designing PGDS inhibitor using the three-dimensional structures.

Prostaglandin D₂ (PGD₂) is synthesized in vivo by PGDS from prostaglandin H₂ (PGH₂). There are two types of PGDS,
15 i.e., brain-type PGDS and hematopoietic PGDS. Hematopoietic PGDS absolutely requires glutathione for the enzymatic reaction while brain-type PGDS also causes the enzymatic reaction in the presence of thiol reagents other than glutathione.

20 PGD₂ is synthesized in central nervous system by brain-type PGDS, and has the function of sleep induction, thermodepression, inhibition of secretion of corpus luteum hormone and control of response of pain and odor. PGD₂ is synthesized in peripheral tissue by hematopoietic PGDS, and
25 is known to have physiological function such as dilation of

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peripheral blood vessel, bronchoconstruction, and inhibition of platelet coagulation and act as an allergic mediator released from mast cells (Lewis, R. A., Soter, N. A., Diamond, P. T., Austen, K. F., Oates, J. A. & Roberts, L. J. Prostaglandin D₂ generation after activation of rat and human mast cells with anti-IgE. J. Immunol., 129, 1627-1631 (1982)). It is reported that allergic reaction is significantly reduced in knockout mouse of prostaglandin D₂ receptor protein (DP receptor) (Matsuoka, T., Hirata, M., Tanaka, H., Takahashi, Y., Murata, T., Kabashima, K., Sugimoto, Y., Kobayashi, T., Ushikubi, F., Aze, Y., Yoshida, N., Honda, Y., Nagai, H. & Narumiya, S. Prostaglandin D₂ as a mediator of allergic asthma. Science, 287, 2013-2017 (2000)). There is another prostaglandin D₂ receptor (CRTH2 receptor) in Th2 lymphocytes, eosinophils, and basophils involved in allergic reaction, which promotes chemotaxis of those inflammatory cells (Hirai, H., Tanaka, K., Yoshie, O., Ogawa, K., Kenmotsu, K., Takamori, Y., Ichimasa, M., Sugamura, K., Nakamura, M., Takano, S., and Nagata, K., Prostaglandin D₂ selectively induces chemotaxis in T helper type 2 cells, eosinophils and basophils via seven-transmembrane receptor CRTH2, J. Exp. Med., 193, 255-261 (2001)). The synthesis of prostaglandin D₂ in mast cells (Urade, Y., Ujihara, M., Horiguchi, Y., Igarashi, M., Nagata, A., Ikai, K. and Hayaishi, O. Mast cells contain

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spleen-type prostaglandin D synthase, J. Biol. Chem., 265, 371-375 (1990)) and human Th2 lymphocytes (Tanaka, K., Ogawa, K., Sugamura, K., Nakamura, M., Takano, S. and Nagata, K., Differential production of prostaglandin D2 by human helper T cell subsets, J. Immunol., 164, 2277-2280 (2000)) is made by hematopoietic PGDS.

If a compound capable of inhibiting the enzymatic activity of PGDS, it would become possible to control PGD₂ synthesis to obtain anti-allergic agent, sleep control agent and anti-obesity agent.

Recently, an attempt to design medicine from three dimensional structure of protein has been made. However, no one has succeeded in determining the three dimensional structure of human hematopoietic PGDS. It is hence difficult to design an inhibitor of human hematopoietic PGDS from the three dimensional structure thereof. It is an object of the present invention to clarify the three dimensional structure of human hematopoietic PGDS to provide a method for designing an inhibitor of human hematopoietic PGDS using the three dimensional structure.

SUMMARY OF THE INVENTION

The inventors has succeeded in preparing crystals of complexes of human hematopoietic PGDS (which has as metal ion calcium ion (referred to as "calcium type" hereinafter) or magnesium ion (referred to as "magnesium type"

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hereinafter)), glutathione (GSH) which is a cofactor of PGDS, and analog of prostaglandin H_2 (PGH_2) which is a substrate of PGDS or several types of inhibitor of PGDS. The inventor has succeeded in clarifying the three dimensional structure of those complex with crystallography technique using X-ray diffraction method for the first time.

The present invention is related to a complex of human calcium type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1 and glutathione which has a three dimensional structure represented by the structural coordinates in Table 1.

The present invention is related to a complex of human magnesium type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1 and glutathione which has a three dimensional structure represented by the structural coordinates in Table 2.

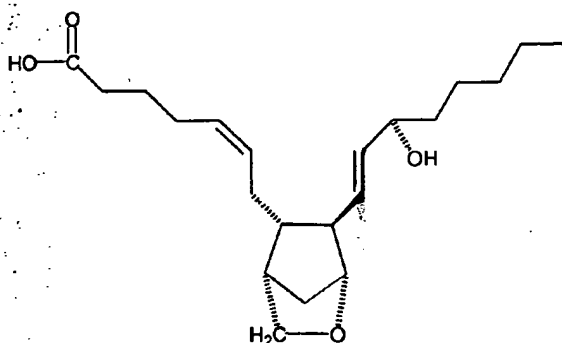
The present invention is related to a complex of human calcium type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1, glutathione and 9,11-dideoxy -9 α , 11 α methanoepoxyprostaglandin F_2 (referred to as "U46" hereinafter) which has a three dimensional structure represented by the structural coordinates in Table 3.

U46 is represented by the formula:

(Formula 1)

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and is an analog of prostaglandin H_2 (PGH_2) which is a substrate of PGDS

The present invention is related to a complex of human
5 magnesium type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1, glutathione and U46 which has a three dimensional structure represented by the structural coordinates in Table 4.

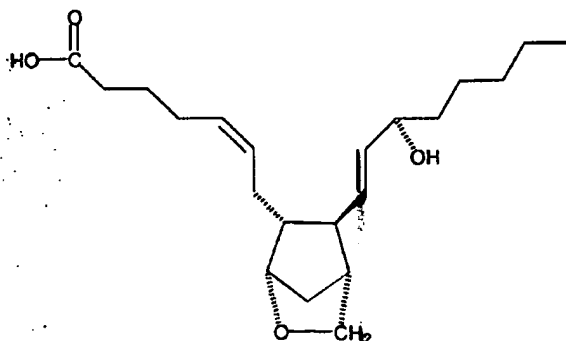
The present invention is related to a complex of human
10 calcium type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1, glutathione and 9,11-dideoxy -9 α ,11 α epoxymetanoprostaglandin F_2 (referred to as "U44" hereinafter) which has a three dimensional structure represented by the structural coordinates in Table 5.

15 U44 is represented by the formula:

(Formula 2)

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and is an analog of prostaglandin H₂ which is a substrate of PGDS

The present invention is related to a complex of human magnesium type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1, glutathione and U44 which has a three dimensional structure represented by the structural coordinates in Table 6.

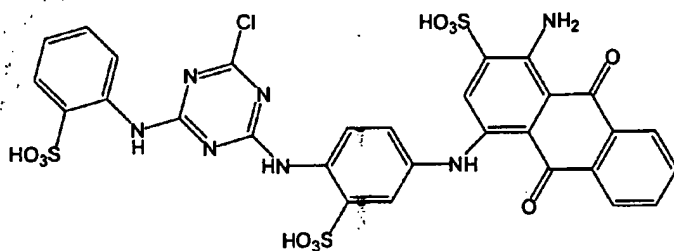
The present invention is related to a complex of human calcium type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1, glutathione and Cibacron Blue(trade mark) (1-amino-4-{4-[4-chloro-6-(2-sulfo-phenylamino)-[1,3,5]triazine-2-ylmethyl]-3-sulfo-phenylamino}-9,10-dioxo-9,10-dihydroanthracene-2-sulfonic acid) which has a three dimensional structure represented by the structural coordinates in Table 7.

Cibacron Blue is represented by the formula:

(Formula 3)

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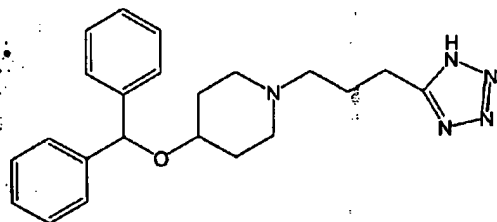


and is known as an inhibitor of PGDS (Thomson, A. M., Meyer, D. J. & Hayes, J. D. Sequence, catalytic properties and expression of chicken glutathione-dependent prostaglandin D₂ synthase, a novel class Sigma glutathione S-transferase. Biochem. J., 333, 317-325 (1998)).

The present invention is related to a complex of human magnesium type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1, glutathione and 4-benzhydryloxy-1-(3-(1H-tetrazol-5-yl)-propyl)piperidine (referred to as "HQL-79" hereinafter) which has a three dimensional structures represented by the structural coordinates in Table 8.

HQL-79 is represented by the formula:

(Formula 4)



and is known to have anti-allergic activity (Matsushita N, Hizue M, Aritake K, Hayashi K, Takada A, Mitsui K, Hayashi M, Hirotsu I, Kimura Y, Tani T and Nakajima H,

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Pharmacological studies on the novel anti-allergic drug
HQL-79: I. Anti-allergic and anti-asthmatic effects in
various experimental models. Japanese Journal of
Pharmacology, 78, 1-10 (1998)).

5 The present invention is further related to use of at
least one structural coordinates selected from the group
consisting of the structural coordinates represented in
Tables 1-8 in selecting a compound inhibiting human
hematopoietic PGDS.

10 The present invention is related to a method for
selecting an inhibitor of human hematopoietic PGDS,
comprising steps of:

(a) providing at least one structural coordinates
selected from the group consisting of the structural
15 coordinates represented in Tables 1-8 which characterizes
an active site of human hematopoietic PGDS;

(b) providing steric structure of a candidate
compound; and

(c) fitting the candidate compound to the active site
20 of human hematopoietic PGDS to select the inhibitor.

The amino acid residues involved in the active site of
human hematopoietic PGDS are Tyr8, Phe9, Asn10, Met11,
Arg12, Gly13, Arg14, Ala15, Glu16, Leu17, Trp39, Pro40,
Glu41, Ile42, Lys43, Gly49, Lys50, Ile51, Pro52, Ile53,
25 His62, Gln63, Ser64, Leu65, Asp93, Thr94, Leu95, Asp96,

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Asp97, Phe98, Met99, Ser100, Cys101, Phe102, Phe103, Trp104,
Ala105, Glu106, Lys107, Lys108, Gln109, Asp110, Val111,
Lys112, Glu113, Gln114, Met115, Phe116, Tyr152, Trp153,
Glu154, Ile155, Leu156, Ser157, Thr158, Thr159, Leu160,
5 Leu161, Val162, Phe163, Thr197, Lys198, and Leu199.

The term "fit" means that a candidate compound is
optimized in energy and configuration to the active site of
human hematopoietic PGDS. A compound is selected in such a
manner that the contact area of a candidate compound with
10 human hematopoietic PGDS is maximum when the compound binds
to the active site of human hematopoietic PGDS, and that
the binding mode between the compound and the active site
of human hematopoietic PGDS is maximum.

Preferably, it is confirmed that the thus selected
15 inhibitor has the inhibiting effect of PGDS by contacting
the inhibitor with hematopoietic PGDS in the presence of
prostaglandin H₂.

In addition, the inhibitor is confirmed whether it has
at least one biological activity selected from the group
20 consisting of anti-allergic activity, sleep control
activity, anti-obesity activity and brain wound healing
activity.

BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1 shows the three-dimensional structure of a
25 complex of human hematopoietic prostaglandin D synthase

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(PGDS) (calcium type) and glutathione. PGDS forms a dimer, and there is a metal ion-binding site in the center of the dimer.

Figure 2 shows PGDS monomer structure viewed from the side of the monomer.

Figure 3 shows a surface structure of PGDS viewed from the same direction as in Figure 2.

Figure 4 is an enlarged view of surface structure of PGDS complexed with calcium, glutathione, and U46. Oxygen atom of cyclopentane ring of U46 forms hydrogen bond with glutathione

Figure 5 shows three-dimensional structure of PGDS complexed with calcium, glutathione and U44. Alpha chain of the substrate analogue is surrounded by Lys107, Lys112 and Lys198 of PGDS which are basic amino acid residues. The residues form salt-bridge with carboxylate of the α chain. In magnesium-type PGDS, similar three-dimensional structure is observed.

Figure 6 shows three dimensional structure of PGDS complexed with magnesium, glutathione and U46.

DETAILED DESCRIPTION OF THE PREFERRED EMBODIMENTS

(1) Human hematopoietic prostaglandin D synthase

The amino acid sequence of human hematopoietic prostaglandin D synthase is known. The method for

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preparing it is also disclosed (Japanese Patent Kokai No. 322773/1997). Although it is possible to obtain the enzyme from human tissue, it is convenient to prepare it using recombinant technique.

5 For example, an expression plasmid (pT7-7hPGDS) which comprises cDNA encoding human hematopoietic prostaglandin D synthase having amino acid sequence of SEQ. ID. NO. 1 under the control of T7 polymerase gene promoter is constructed (Japanese Patent Kokai No. 322773/1997). *Escherichia coli* BL21 (DE-3) is transformed with the expression plasmid using modified calcium chloride method (Inoue, et al., Gene 10 96:23-28 (1990)). *Escherichia coli* pYK1 transformed with the expression plasmid is deposited under accession number FERM BP-5489 in National Institute of Advanced Industrial Science and Technology.

15 *Escherichia coli* pYK1 is cultured in LB medium (containing 50 μ g/ml of ampicillin) at 37 °C overnight. IPTG (isopropylthio- β -D-galactoside) is then added to final concentration of 0.4mM and *Escherichia coli* pYK1 is further cultured for additional 4 to 6 hours.

20 After the completion of cultivation, the bacteria is fractured by ultrasonic, centrifuged at 13,000 rpm at 4 °C for 15 minutes to remove precipitates. Fractionation is effected with ammonium sulfate. Fraction of 40% to 60% saturation of ammonium sulfate is obtained and dialyzed

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against 50 mM sodium phosphate buffer. The dialyzed solution is applied to Glutathione Sephalose 4B column and purified by affinity chromatography.

5 (II) Crystal of human hematopoietic prostaglandin D synthase complex

Crystallization of protein utilizes a property of protein that it is deposited under some conditions as a crystal when protein is made from dissolving condition to
10 non-dissolving condition by adding a precipitating agent to a solution of protein of interest, or by reducing amount of solution by vaporizing solvent.

The inventors have found that human hematopoietic PGDS complex is successfully crystallized with hanging drop
15 vapor diffusion method. The hanging drop vapor diffusion method is a method wherein a mixed solution of protein solution with a precipitating solution is hanged up on a glass plate using surface tension and the solution is enclosed with another precipitating solution having higher
20 concentration in a sealed space to form a crystal of the protein. Due to vapor diffusion, the concentration of the precipitating agent is gradually higher to obtain a crystal. When large crystal is required, a crystal obtained in a first crystallization and having a size of about 0.01 mm is
25 selected and re-crystallized again with macro-seeding

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method (Stura, E. A. & Wilson, L. A. Applications of the streak seeding technique in protein crystallization. J. of Crystal Growth, 110, 270-282 (1991).) to obtain a crystal having size of about 0.3 x 0.3 x 1.5 mm which is proper for X-ray diffraction experiment.

The conditions for preparing of eight human hematopoietic PGDS complexes are described hereinafter.

(1)Complex of human hematopoietic PGDS with calcium and glutathione

10 Composition:

		Internal Sol.	External Sol.
Precipitant-	PEG 6000	14%	16%
ing agent			
Buffer	Tris buffer	50mM	100mM
15 Admixture	Glutathione	5mM	10mM
	dithiothreitol	5mM	10mM
	Calcium chloride	2.5mM	5mM
	Dioxane	1%	2%
Protein	PGDS	5mg/mL	-

20 Temperature:20°C, pH:8.4

(2)Complex of human hematopoietic PGDS with magnesium and glutathione

composition:

25 Internal Sol. External Sol.

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5	Precipitant-	PEG 6000	14%	16%
	ing agent			
	Buffer	Tris buffer	50mM	100mM
	Admixture	Glutathione	5mM	10mM
		dithiothreitol	5mM	10mM
		Magnesium chloride	2.5mM	5mM
		Dioxane	1%	2%
	Protein	PGDS	5mg/mL	-

Temperature: 20°C, pH: 8.4

10

(3) Complex of human hematopoietic PGDS with calcium, glutathione and 9,11-dideoxy -9 α , 11 α - methanoepoxyprostaglandine F_{2 α} (U46)

Composition:

15			Internal Sol.	External Sol.
	Precipitant-	PEG 6000	14%	16%
	ing agent			
	Buffer	Tris buffer	50mM	100mM
	Admixture	Glutathione	5mM	10mM
20		dithiothreitol	5mM	10mM
		Calcium chloride	2.5mM	5mM
		Dioxane	1%	2%
		U46	10mM	-
	Protein	PGDS	5mg/mL	-

25 Temperature: 20°C, pH: 8.4

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(4)Complex of human hematopoietic PGDS with magnesium, glutathione and 9,11-dideoxy -9 α ,11 α - methanoepoxyprostaglandine F_{2 α} (U46)

5 Composition:

		Internal Sol.	External Sol.
	Precipitatat-		
	PEG 6000	14%	16%
	ing agent		
	Buffer	Tris buffer	50mM
			100mM
10	Admixture	Glutathione	5mM
			10mM
		dithiothreitol	5mM
			10mM
		Magnesium chloride	2.5mM
			5mM
		Dioxane	1%
			2%
		U46	10mM
			-
15	Protein	PGDS	5mg/mL
			-

• Temperature:20°C, pH:8.4

(5)Complex of human hematopoietic PGDS with calcium, glutathione and 9,11-dideoxy -9 α ,11 α - epoxymethanoprostaglandine F_{2 α} (U44)

20

Composition:

		Internal Sol.	External Sol.
	Precipitatat-		
	PEG 6000	14%	16%
	ing agent		
25	Buffer	Tris buffer	50mM
			100mM

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5	Admixture	Glutathione	5mM	10mM
		dithiothreitol	5mM	10mM
		Calcium chloride	2.5mM	5mM
		Dioxane	1%	2%
		U46	5mM	-
	Protein	PGDS	5mg/mL	-

Temperature: 20°C, pH: 8.4

(6) Complex of human hematopoietic PGDS with magnesium, glutathione and 9,11-dideoxy -9 α , 11 α - epoxymethanoprostaglandine F₂ α (U44)

Composition:

		Internal Sol.	External Sol.
15	Precipitatat-		
	PEG 6000	14%	16%
	ing agent		
	Buffer	Tris buffer	50mM
			100mM
	Admixture	Glutathione	5mM
			10mM
		dithiothreitol	5mM
			10mM
		Magnesium chloride	2.5mM
			5mM
20		Dioxane	1%
			2%
		U44	5mM
			-
	Protein	PGDS	5mg/mL
			-

Temperature: 20°C, pH: 8.4

(7) Complex of human hematopoietic PGDS with calcium,

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glutathione and Cibacron Blue (trade mark) (1-amino-4-{4-[4-chloro-6-(2-sulfo-phenylamino)-[1,3,5]triazine-2-ylmethyl]-3-sulfo-phenylamino}-9,10-dioxo-9,10-dihydro-anthracene-2-sulfonic acid)

5 Composition:

		Internal Sol.	External Sol.
Precipitatat-	PEG 6000	14%	16%
ing agent			
Buffer	Tris buffer	50mM	100mM
10 Admixture	Glutathione	5mM	10mM
	dithiothreitol	5mM	10mM
	Calcium chloride	2.5mM	5mM
	Dioxane	1%	2%
	Cibacron Blue	1mM	-
15 Protein	PGDS	5mg/mL	-

Temperature: 20°C, pH: 8.4

(8) Complex of human hematopoietic PGDS with calcium, glutathione and 4-benzhydryloxy-1-{3-(1H-tetrazol-5-yl)-propyl}piperidine (HQL-79)

20

Composition:

		Internal Sol.	External Sol.
Precipitatat-	PEG 6000	14%	16%
ing agent			
25 Buffer	Tris buffer	50mM	100mM

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5	Admixture	Glutathione	5mM	10mM
		dithiothreitol	5mM	10mM
		Calcium chloride	2.5mM	5mM
		Dioxane	1%	2%
		HQL-79	saturated	-
	Protein	PGDS	5mg/mL	-

Temperature: 20°C, pH: 8.4

10 (III) Three-dimensional coordinate of human hematopoietic PGDS complex

Three-dimensional structure of human hematopoietic PGDS complex is clarified using X-ray crystallography from the crystal of human hematopoietic PGDS complex obtained from (II).

15 Data collection was carried out for mercury derivative crystal of human hematopoietic PGDS of the calcium type in Spring-8 RIKEN beam line BL45XD in consideration of anomalous dispersion effect. Data collection was carried out using synchrotron radiation lights of three wavelengths
20 of 1.009 Å, 1.04 Å and 1.10 Å to calculate eight positions of mercury from the analysis of Patterson function. The position is made precise using the program MLPHARE (Otwinowski, Z. in Proceedings of CCP4 Study Weekend, Isomorphous Replacement and Anomalous Scattering, edited by
25 Sawyer, L., Issacs, N., and Bailey, S. [Science and

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Engineering Research Council (England) Daresbury Lab.,
 Warrington, U.K.], pp. 80-86 (1993)) to obtain electron
 density of the enzyme. Enzyme model was constructed on
 graphics workstation to obtain an enzyme model of human
 5 hematopoietic PGDS of the calcium type in high accuracy
 using a refinement program CNS (Brunger, A. T., Adams, P.
 D., Clore, G. M., DeLano, W. L., Gros, P., Grosse-Kunstleve,
 R. W., Jiang, J. S., Kuszewski, J., Nilges, M., Pannu, N.
 S., Read, R. J., Rice, L. M., Simonson, T. & Warren, G. L.
 10 Crystallography & NMR system: A new software suite for
 macromolecular structure determination. Acta Cryst., D54,
 905-921 (1998)).

The other structural model was obtained in high
 accuracy with the program CNS using the calcium type model
 15 firstly obtained as the search model.

Crystallographic data obtained for the crystals
 prepared in (II)(1) to (II)(8) are as follows:

Crystal	(1)	(2)	(3)	(4)
20 Space group	P2 ₁	P2 ₁	P2 ₁	P1
Resolution(Å)	37.3-1.8	30.9-1.7	37.3-2.0	33.8-1.2
No. of water molecules	1089	983	744	1587
R _{cryst} (%)	19.3	21.0	20.6	18.0
R _{free} (%)	22.6	24.1	25.2	19.1
25 R.m.s.deviation of				

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	bond length(Å)	0.005	0.006	0.006	0.006
	Bond angles(deg.)	1.1	1.0	1.0	1.2
	dihedral angles(deg.)	20.3	20.1	20.2	20.6
	Average B(Å ²)	18.7	24.5	18.2	14.9
5	<u>Average B of GSH(Å²)</u>	<u>17.7</u>	<u>27.2</u>	<u>20.8</u>	<u>10.0</u>

Crystal	(5)	(6)	(7)	(8)
Space group	P2 ₁	P2 ₁	P2 ₁	P1
10 Resolution(Å)	37.4-1.8	29.0-2.0	91.6-2.1	500-1.45
No. of water molecules	858	1639	858	1398
R _{cryst} (%)	21.2	17.8	20.3	19.2
R _{free} (%)	24.7	23.0	25.7	20.7
R.m.s. deviation of				
15 bond length(Å)	0.006	0.006	0.007	0.012
Bond angles(deg.)	1.0	1.1	1.1	1.3
dihedral angles(deg.)	20.4	20.6	20.1	20.1
Average B(Å ²)	22.8	19.5	22.4	14.4
<u>Average B of GSH(Å²)</u>	<u>23.6</u>	<u>15.1</u>	<u>44.8</u>	<u>11.6</u>

20.

Table 1 represents the structural coordinates of the complex of human hematopoietic PGDS with calcium and glutathione; Table 2 represents the structural coordinates of the complex of human hematopoietic PGDS with magnesium and glutathione; Table 3 represents the structural

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coordinates of the complex of human hematopoietic PGDS with calcium, glutathione and 9,11-dideoxy -9 α ,11 α -methanoepoxyprostaglandine F₂_a (U46); Table 4 represents the structural coordinates of the complex of human hematopoietic PGDS with magnesium, glutathione and 9,11-dideoxy -9 α ,11 α -methanoepoxyprostaglandine F₂_a (U46); Table 5 represents the structural coordinates of the complex of human hematopoietic PGDS with calcium, glutathione and 9,11-dideoxy -9 α ,11 α -epoxymethanoprostaglandine F₂_a (U44); Table 6 represents the structural coordinates of the complex of human hematopoietic PGDS with calcium, glutathione and 9,11-dideoxy -9 α ,11 α -epoxymethanoprostaglandine F₂_a (U44); Table 7 represents the structural coordinates of the complex of human hematopoietic PGDS with calcium, glutathione and Cibacron Blue (trade mark); Table 8 represents the structural coordinates of the complex of human hematopoietic PGDS with magnesium, glutathione and 4-benzhydryloxy-1-(3-(1H-tetrazol-5-yl)-propyl)piperidine (HQL-79).

Each table represents three-dimensional structural coordinates according to the format of Protein Data Bank (<http://rcsb.org/pdb/>, USA). "ATOM" at the first column indicates that the row describes atom coordinates; the second column indicates the atom number; the third column

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indicates the atom type in the amino acid residue or the like, for example, carbonyl carbon atom is represented by C, and carbonyl oxygen atom is represented by O,; the fourth column indicates the amino acid residue or the like; the fifth column indicates the class of molecule; the sixth column indicates the amino acid number; the seventh, eighth, and ninth columns indicate coordinates of the atom (in Å for X-axis, Y-axis, and Z-axis directions in the order); the tenth column indicates the occupancy of the atom (in the present invention 1.00 for all atoms); and the eleventh column indicates the temperature factor of the atom. The twelveth column indicates the class of molecule like the fifth column.

15 (IV) Three-dimensional structure and binding site of human hematopoietic PGDS complex.

(1) Complex of human hematopoietic PGDS with calcium and glutathione

Prostaglandin D synthase form a dimer and calcium ion exists in the center of the dimer (see Fig.1). Calcium has no influence on the glutathione binding, but increases the reaction rate of PGDS enzyme. Glutathione binds to Tyr8, Arg14, Trp39, Gly49, Lys50, Ile51, Pro52, Gln63 and Ser64 of PGDS.

25 (2) Complex of human hematopoietic PGDS with magnesium and

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glutathione

In accordance with the change of metal ion in the center of the dimer from calcium ion to magnesium ion, coordination structure of water molecule to the metal ion is significantly changed. Magnesium increases the affinity of glutathione to PGDS by more than 3 times.

(3) Complex of human hematopoietic PGDS with calcium, glutathione and 9,11-dideoxy -9 α , 11 α - methanoepoxyprostaglandine F_{2 α} (U46)

In the complex, there exists calcium ion in the center of the dimer as in (1). In addition, substrate analog, U46, binds to PGDS. U46 binds to Tyr8, Gly3, Arg14, Gln36, Trp104, Gln36, Trp104, Gln109, Lys112, Tyr152, Lys198, and Leu199 of PGDS, and GSH. Carboxyl group of U46 is hydrogen bonded to either of Gln109, Lys112, or Lys198 of PGDS. Oxygen atom at C11 site of U46 is positioned at 4.6Å from S atom of GSH. The ω chain of U46 approaches Tyr152 existing in the deepest portion of substrate binding site to van der Waals contact distance.

(4) Complex of human hematopoietic PGDS with magnesium, glutathione and 9,11-dideoxy -9 α , 11 α - methanoepoxyprostaglandine F_{2 α} (U46)

The structure of the complex differs from that of (3) in that magnesium ion exists in the center of the dimer.

Although the α chain of U46 is positioned near Gln109,

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Lys112 and Lys198 of PGDS, it is not hydrogen bonded but is in van der Waals contact. Oxygen atom at 11 site of U46 is hydrogen bonded to Gln36 of PGDS through water molecule. The OH group in the ω chain of U46 is hydrogen bonded to rotated Arg14 and the ω chain is out of the pocket. Ether which is a solvent for U46 binds at the aperture between Trp104 of PGDS and U46 molecule.

(5) Complex of human hematopoietic PGDS with calcium, glutathione and 9,11-dideoxy -9 α , 11 α - epoxymethanoprostaglandine $F_{2\alpha}$ (U44)

The complex differs from that of (1) to (4) in that a substrate analog U44 binds to PGDS. In the calcium-binding structure, although the binding site of U44 is the same as that of U46, the manner of hydrogen bonding differs.

Although they are both in the calcium-binding form, being different from U46, α -chain of U44 is hydrogen bonded with to all of Gln109, Lys112, and Lys198 of PGDS, and oxygen atom at 9 site is hydrogen bonded through water to Gln36. The α -chain of U44 is about 5 Å apart from back Tyr152, differing from the structure of (3).

(6) Complex of human hematopoietic PGDS with magnesium, glutathione and 9,11-dideoxy -9 α , 11 α - epoxymethanoprostaglandine $F_{2\alpha}$ (U44)

Although this complex is identical with (5) in that they are complexes with substrate analog U44, it is

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different from (5) in that the metal ion positioned in the center of dimer is magnesium ion.

(7) Complex of human hematopoietic PGDS with calcium, glutathione and Cibacron Blue (trade mark)

5 The complex differs from the above six structures in that it is a complex with an inhibitor Cibacron Blue. Metal ion in the center of the dimer is calcium. Cibacron Blue binds to Phe9, Gly10, Gly13, Arg14, Gln36, Met99, Ser100, Trp104, Glu106, Lys107, Gln109, Lys112, Tyr152, 10 Cys156, Lys198, and Leu199 of PGDS, and GSH

(8) Complex of human hematopoietic PGDS with magnesium, glutathione and 4-benzhydryloxy-1-{3-(1H-tetrazol-5-yl)-propyl}piperidine (HQL-79)

15 The complex is different from (1) to (6) in that it is a complex with an inhibitor HQL-79, and an inhibitor different from (7) is used. Magnesium ion is bonded in the center of the dimer. Induce-fit phenomenon is caused due to the binding of HQL-79, and space group is changed from P2₁ to P1. HQL-79 binds to Tyr8, Phe9, Arg14, Met99, 20 Phe102, Trp104, Tyr152, Ile155, Thr159, Phe163, and Leu199 of PGDS and GSH.

(V) Use of three dimensional coordinates for preparing inhibitor of human hematopoietic prostaglandin D synthase

25 A compound capable of inhibiting human hematopoietic

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PGDS can be selected using three-dimensional coordinates of Tables 1 to 8.

The present invention is related to a method for selecting an inhibitor of human hematopoietic PGDS, comprising steps of:

(a) providing at least one of these structural coordinates selected from the group consisting of the structural coordinates represented in Tables 1-8 which characterizes an active site feature of human hematopoietic PGDS;

(b) providing steric structure of a candidate compound; and

(c) fitting the candidate compound to the active site of human hematopoietic PGDS to select the inhibitor.

The amino acid residues involved in the active site of human hematopoietic PGDS are Tyr8, Phe9, Asn10, Met11, Arg12, Gly13, Arg14, Ala15, Glu16, Leu17, Trp39, Pro40, Glu41, Ile42, Lys43, Gly49, Lys50, Ile51, Pro52, Ile53, His62, Gln63, Ser64, Leu65, Asp93, Thr94, Leu95, Asp96, Asp97, Phe98, Met99, Ser100, Cys101, Phe102, Phe103, Trp104, Ala105, Glu106, Lys107, Lys108, Gln109, Asp110, Val111, Lys112, Glu113, Gln114, Met115, Phe116, Tyr152, Trp153, Glu154, Ile155, Leu156, Ser157, Thr158, Thr159, Leu160, Leu161, Val162, Phe163, Thr197, Lys198, and Leu19

Based on the three-dimensional structure information,

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commercially available compound is one by one minimized in energy using various programs so that the binding to the active site of the enzyme occurs in the most appropriate orientation. This procedure is automatically effected for all commercially available compounds to compare free energy to select compound which readily bind to the active site of the enzyme. Compound thus obtained is used as basic backbone, and more stable derivative is designed to synthesize more stable compound to develop new inhibitor of the enzyme.

It is preferred to design inhibitor using computer. For example, Indigo 2, a workstation supplied by Silicon Graphics, Inc., is suitable as a computer used for designing inhibitors. However, the computer is not limited to this one, and any computer may be used so long as it is tuned to run an appropriate program. Likewise, there is no particular limitation on the computer storage medium. For example, Insight II, a computer program commercially available from Accelrys, Inc. may be used as a program for designing. In particular, a program Ludi or DOCK, a module of Insight II specially prepared for such purposes, may be used alone or in combination to facilitate identification, searching, evaluation, or designing.

In designing of inhibitor, there are conceptually two steps. The first step is to find a compound which serves

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as a starting point for drug design, known for those skilled in the art as a lead compound. The next step is optimization of the lead compound wherein compounds having better properties as medicines, for example, having better activity, having better pharmacokinetics, or having less toxicities and side effects are sought starting from the lead compound.

The step in which a lead compound is found using the structure coordinates of the PGDS complex provided by the present invention is achieved, for example, using a database in a computer into which structures of plural compounds have been entered, by a method in which interactions between three-dimensional structures of a compound in the database and PGDS are sorted out in a visual manner one after another, or by a method in which amplitudes of binding energy are calculated one after another using a computer and compounds which stably bind to PGDS are found from the database. Although it is preferred that the database of compound's structures contains determined three-dimensional structure coordinates entered therein, for low molecular weight compounds, it does not have to be a database of three-dimensional structure coordinates, because such low molecular weight compounds may change their conformations relatively freely, and also because three-dimensional structure coordinates for each

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conformation can be derived by calculations in a relatively short time. In the latter cases, information for chemical covalent bonds of low molecular weight compounds are entered into the database.

5 Specifically, in the visual method, PGDS complexes are firstly displayed on a computer screen according to the structure coordinates of the present invention. In this step, although a three-dimensional representation may be made on the computer screen using, for example, Crystal Eye
10 as described above, visual examinations can also be achieved without using such a three-dimensional representation.

Chemical interactions to be considered include electrostatic interaction, hydrophobic interaction,
15 hydrogen bonding, van der Waals interaction, and the like. Thus, the structure should be comprehensively examined whether it is favorable for interactions, for example, so that functional groups which tend to bear negative charge such as carboxyl group, nitro group, and halogens interact
20 with amino acid residues in PGDS having positive charge such as lysine, arginine, and histidine, so that functional groups which tend to bear positive charge such as amino, imino, and guanidyl groups interact with amino acid residues in PGDS having negative charge such as glutamic
25 acid and aspartic acid, so that hydrophobic functional

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groups such as aliphatic groups and aromatic groups interact with hydrophobic amino acid residues such as alanine, leucine, isoleucine, valine, proline, phenylalanine, tryptophan and methionine, so that functional groups involved in hydrogen bonding such as hydroxyl and amide groups can form hydrogen bonds with backbone or side chain portions of PGDS, so that binding between the compound and PGDS causes no steric hindrance, and so that empty spaces are filled to minimize such empty spaces and maximize van der Waals interaction. Thus, electrostatic interaction, hydrophobic interaction, van der Waals interaction, hydrogen bonding, and other factors are visually and comprehensively considered to finally determine whether or not the compound is suitable as a lead compound.

In the method by energy evaluation with a computer, the energy of binding between a compound and PGDS is determined by molecular force field calculations. Such calculations are applied to each compound in the database to find a certain compound which may serve as a lead compound capable of stable binding. As a molecular force field used in the calculations, for example, CVFF, AMBER force field optimized for proteins, which is contained in DISCOVER module of Insight II program may be used. In addition, some computer programs like Ludi in Insight II

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can automatically output candidates for lead compound when three-dimensional structure coordinates of interacting amino acid residues in a protein molecule are given, and such programs may also be applied to the method of present invention.

Furthermore, the visual examinations and the examination considering energy are not strictly sorted out from each other, and both techniques may be used in combination as appropriate.

The next step, in which optimization of the lead compound is conducted using the structure coordinates of the PGDS complex is used for the purpose of, where a lead compound which binds to PGDS has already been found by the above method or separately found in an experimental manner, optimizing the lead compound to obtain a better compound, for example, a compound having higher biological activities as an inhibitor or a compound having a structure favorable for oral administration as a medicine. It becomes possible only after a precise picture of chemical bonding between the lead compound and PGDS has been elucidated to directly find a site which is not optimal for interactions between the lead compound and PGDS and to design a new compound having an optimal functional group at that site, thereby enabling to design a more optimized compound.

For visual examinations with a computer, a model of

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the complex between the lead compound and PGDS is firstly displayed on a computer screen by entering the three-dimensional structure coordinates of the lead compound and the structure coordinates of PGDS provided by the present invention into a computer on which a computer program expressing three-dimensional coordinates of molecules runs or into a storage medium of the computer. In this step, although a three-dimensional representation may be made on the computer screen using, for example, Crystal Eye as described above, visual examinations can also be achieved without using such a three-dimensional representation. It is a logical designing of a compound to modify the lead compound so as to yield a compound more favorably interacting with PGDS or a compound having better pharmacokinetics while retaining the interactions.

Chemical interactions to be considered are the same as those in the step to find a lead compound, and a new compound having better properties as an inhibitor is finally designed starting from the lead compound.

In the method by energy evaluation with a computer, the energy of binding between a new compound designed from the lead compound and PGDS is determined by molecular force field calculations to judge the validity of the design. In addition, it is also possible to use a method in which other molecules such as solvent molecules are additionally

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included in the model and the free energy is determined using molecular dynamics to derive a compound capable of stable binding. As a molecular force field used in the calculations, for example, CVFF, AMBER force field optimized for proteins, which is contained in DISCOVER module of Insight II program may be used.

Furthermore, the visual examinations and the method by energy evaluations may be used in combination as appropriate.

After a candidate compound for inhibitor of hematopoietic PGDS is thus selected, the selected compound is contacted with the enzyme in the presence of the substrate (prostaglandin H₂) to confirm an ability of the compound to inhibit the enzymatic activity (Shimizu, T., Yamamoto, S., and Hayaishi, O. (1979). Purification and properties of prostaglandin D synthase from rat brain. J. Biol. Chem. 254, 5222-5228). The measurement of the enzymatic activity is, for example, carried out as follows:

The substrate [1-¹⁴C]prostaglandin(PG)H₂ is prepared by reacting [1-¹⁴C]arachidonic acid with cyclooxygenase. Since PGH₂ is easily decomposed in aqueous solution(half-life: about 5 minutes), it is dried and stored at a low temperature(-80°C). The enzymatic reaction is carried out by injecting with microsyringe 1 μl of PGH₂ solution (acetone or nonvolatile diethleneglycol solution) to 50 μ

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1 of 0.1 M phosphate buffer (pH 7.5) containing 1mM
glutathione and the enzyme. After the reaction is effected
for 30~60 seconds, the reaction is quenched by adding 300
μ l of ice-cooled ether/methanol/0.1M citric acid
5 mixture(20:4:1 v/v/v), and the substrate and the reaction
product are extracted with ether under acidic condition.
Anhydrous sodium sulfate is then added to the reaction
solution to remove water. An aliquot (about 50 μ l) of
organic layer is applied on silica gel thin layer in a cool
10 room (about 4°C) and silica gel thin layer chromatography
(development solvent: ether/methanol/acetic acid (9:2:0.1))
is carried out in a freezer (-20 °C). After the
development, radioactivity of PGD₂ fraction and other
fraction are measured and the enzyme activity is calculated
15 from the ratio of conversion to PGD₂.

Alternatively, enzyme reaction is carried out using
commercially available non-labeled PGH₂. After the
reaction, PGH₂ is decomposed to 12(S)-hydroxy-8,10-trans-5-
cis-heptadecatrienolic acid with the treatment by FeCl₂
20 before quantifying with reverse phase HPLC using 11-β-PGE₂
as an internal standard or commercially available ELISA to
quantify PGD₂.

Since inhibitor of hematopoietic PGDS can be anti-
allergic agent, sleep control agent, anti-obesity agent,
25 and brain wound healing agent pharmacological activity of

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the inhibitor is measured as each medicine.

A method for measuring pharmacological activity as anti-allergic agent is described in Fugner A, Bechtel W. D., Kuhn, F. J. and Mierau, J. In vitro and in vivo studies of the non-sedating antihistamine epinastine. *Arzneimittelforschung*, 38, 1446-1453 (1988); Kamei, C., Izushi, K., Adachi, Y., Shimazawa, M. and Tasaka, K. Inhibitory effect of epinastine on the type II-IV allergic reactions in mice, rats and guinea pigs. *Arzneimittelforschung*, 41, 1150-1153 (1991). Activity of anti-allergic agent is measured as follows: Candidate compound for prostaglandin D synthase inhibitor is administered to animal or cell. Allergic reaction in animal or the production of prostaglandin D₂ from cell is measured to evaluate the activity in individual or the activity in cell of candidate compound. Alternatively, for example, any allergen is administered to animal before candidate compound for prostaglandin D synthase inhibitor is administered and systemic allergic reaction of the animal is observed to evaluate efficacy of the candidate compound. Alternatively, for example, any allergen is administered to animal to put the animal in allergic condition. Cells are collected from the animal, and the candidate compound of prostaglandin D synthase inhibitor is added to the cells in vitro. The amount of prostaglandin

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D₂ prepared by the stimulation of cell with allergen is measured to evaluate of efficacy of the candidate compound.

A method for measuring pharmacological activity as sleep control agent is described in Huang, Z.-H., Qu, W.-M.,
5 Li, W.-D., Mochizuki, T., Eguchi, N., Watanabe, T., Urade, Y. & Hayaishi, O. Arousal effect of orexin A depends on activation of the histaminergic system. *Proc. Natl. Acad. Sci. USA*, 98, 9965-9970 (2001). For example, the activity is measured as follows: When prostaglandin D synthase
10 inhibitor is administered in ventricle of the brain of mouse, significant sleep disturbance occurs. On the other hand, when prostaglandin D₂ is administered in the ventricle of the brain of mouse, sleep is induced. Accordingly, the candidate compound of prostaglandin D
15 synthase inhibitor is administered to animal and sleep condition is observed to evaluate medical efficacy of the candidate compound. The measurement of sleep condition of animal is, for example, carried out by measuring brain wave, electromyogram, activity, feeding and water-drinking amount,
20 temperature, etc. from time to time.

A method for measuring pharmacological activity as anti-obesity agent is described in Ikeda H, Taketomi S, Sugiyama Y, Shimura Y, Sohda T, Meguro K & Fujita T. Effects of pioglitazone on glucose and lipid metabolism in
25 normal and insulin resistant animals. *Arzneimittelforschung*,

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40, 156-162 (1990) and Sohda T, Mizuno K, Momose Y, Ikeda H, Fujita T & Meguro K. Studies on anti-diabetic agents. 11. Novel thiazolidinedione derivatives as potent hypoglycemic and hypolipidemic agents. J. Med. Chem., 35, 2617-2626 (1992).

The measurement of pharmacological activity as anti-obesity agent is carried out as follows: Prostaglandin D synthase inhibitor candidate is administered to animal and activity of the candidate compound in individual is measured by measuring obesity condition of animal. For example, high fatty food is given to animal and the candidate compound of prostaglandin D synthase inhibitor is then administered to animal. Obesity condition of animal is, for example, estimated by measuring body weight, active mass, feeding amount, fat weight, biochemical value in blood, etc. from time to time.

The measurement of activity of brain wound healing agent in individual is carried out as follows: Medical efficacy of the candidate compound is measured by administering the candidate compound of prostaglandin D synthase inhibitor to animal and measuring the degree of brain wound healing. For example, it is measured by administering the candidate compound of prostaglandin D synthase inhibitor to traumatic cerebral cortex wound (Stab wound) model (Salhia B et al, Brain Res., 888:87-97, 2000;

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Asahi M., et al., J. Neurosci., 21:7724-7732, 2001; Garcia
de Yebenes E., et al., J. Neurochem., 73:812-1999). The
measurement of brain wound healing is effected by measuring
for example, amount of behavior, immunohistochemical
5 staining, amount of expressed gene.

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Table 1

Three-dimensional structural coordinate of the complex of
human hematopoietic PGDS with calcium and glutathione

5	ATOM 4966	N	TYR A	8	-2.182	-4.051	33.067	1.00	13.69	A
	ATOM 4967	CA	TYR A	8	-0.772	-4.337	33.302	1.00	13.75	A
	ATOM 4968	CB	TYR A	8	0.013	-3.029	33.442	1.00	12.77	A
	ATOM 4969	CG	TYR A	8	1.519	-3.203	33.467	1.00	11.97	A
	ATOM 4970	CD1	TYR A	8	2.186	-3.810	32.407	1.00	11.66	A
10	ATOM 4971	CE1	TYR A	8	3.576	-3.936	32.403	1.00	11.17	A
	ATOM 4972	CD2	TYR A	8	2.279	-2.725	34.535	1.00	11.40	A
	ATOM 4973	CE2	TYR A	8	3.666	-2.843	34.545	1.00	11.23	A
	ATOM 4974	CZ	TYR A	8	4.307	-3.447	33.475	1.00	11.71	A
	ATOM 4975	OH	TYR A	8	5.680	-3.555	33.475	1.00	12.03	A
15	ATOM 4976	C	TYR A	8	-0.651	-5.143	34.588	1.00	14.05	A
	ATOM 4977	O	TYR A	8	-1.650	-5.413	35.253	1.00	14.34	A
	ATOM 4978	N	PHE A	9	0.569	-5.539	34.932	1.00	14.40	A
	ATOM 4979	CA	PHE A	9	0.793	-6.283	36.165	1.00	15.06	A
	ATOM 4980	CB	PHE A	9	2.198	-6.887	36.177	1.00	15.16	A
20	ATOM 4981	CG	PHE A	9	2.369	-8.046	35.234	1.00	16.21	A
	ATOM 4982	CD1	PHE A	9	3.275	-7.974	34.180	1.00	16.15	A
	ATOM 4983	CD2	PHE A	9	1.633	-9.214	35.406	1.00	16.28	A
	ATOM 4984	CE1	PHE A	9	3.450	-9.050	33.307	1.00	16.56	A
	ATOM 4985	CE2	PHE A	9	1.797	-10.299	34.540	1.00	16.94	A
25	ATOM 4986	CZ	PHE A	9	2.708	-10.215	33.490	1.00	16.76	A

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	ATOM 4987	C	PHE A	9	0.644	-5.318	37.339	1.00	15.24	A
	ATOM 4988	O	PHE A	9	0.482	-4.111	37.139	1.00	14.55	A
	ATOM 4989	N	ASN A	10	0.692	-5.847	38.559	1.00	15.45	A
	ATOM 4990	CA	ASN A	10	0.577	-5.003	39.742	1.00	15.61	A
5	ATOM 4991	CB	ASN A	10	-0.020	-5.775	40.925	1.00	16.21	A
	ATOM 4992	CG	ASN A	10	-0.106	-4.926	42.189	1.00	16.84	A
	ATOM 4993	OD1	ASN A	10	-0.304	-3.707	42.124	1.00	17.30	A
	ATOM 4994	ND2	ASN A	10	0.032	-5.566	43.344	1.00	17.59	A
	ATOM 4995	C	ASN A	10	1.940	-4.458	40.125	1.00	15.68	A
10	ATOM 4996	O	ASN A	10	2.594	-4.955	41.040	1.00	15.31	A
	ATOM 4997	N	MET A	11	2.371	-3.438	39.396	1.00	15.55	A
	ATOM 4998	CA	MET A	11	3.644	-2.784	39.650	1.00	15.24	A
	ATOM 4999	CB	MET A	11	4.823	-3.726	39.351	1.00	17.25	A
	ATOM 5000	CG	MET A	11	4.880	-4.298	37.949	1.00	19.23	A
15	ATOM 5001	SD	MET A	11	6.385	-5.318	37.662	1.00	22.67	A
	ATOM 5002	CE	MET A	11	5.752	-6.968	37.938	1.00	21.71	A
	ATOM 5003	C	MET A	11	3.705	-1.543	38.772	1.00	14.23	A
	ATOM 5004	O	MET A	11	2.864	-1.363	37.894	1.00	13.37	A
	ATOM 5005	N	ARG A	12	4.671	-0.669	39.031	1.00	13.48	A
20	ATOM 5006	CA	ARG A	12	4.804	0.537	38.227	1.00	12.43	A
	ATOM 5007	CB	ARG A	12	5.841	1.480	38.844	1.00	12.14	A
	ATOM 5008	CG	ARG A	12	5.472	1.978	40.246	1.00	12.08	A
	ATOM 5009	CD	ARG A	12	6.475	3.012	40.757	1.00	11.93	A
	ATOM 5010	NE	ARG A	12	7.833	2.474	40.769	1.00	12.08	A
25	ATOM 5011	CZ	ARG A	12	8.301	1.623	41.680	1.00	12.27	A

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	ATOM	5012	NH1	ARG	A	12	7.520	1.210	42.671	1.00	12.04	A
	ATOM	5013	NH2	ARG	A	12	9.550	1.174	41.589	1.00	11.83	A
	ATOM	5014	C	ARG	A	12	5.232	0.080	36.838	1.00	12.15	A
	ATOM	5015	O	ARG	A	12	4.517	0.285	35.858	1.00	12.05	A
5	ATOM	5016	N	GLY	A	13	6.393	-0.563	36.770	1.00	12.02	A
	ATOM	5017	CA	GLY	A	13	6.898	-1.068	35.509	1.00	11.77	A
	ATOM	5018	C	GLY	A	13	6.769	-0.128	34.328	1.00	11.54	A
	ATOM	5019	O	GLY	A	13	6.967	1.080	34.449	1.00	11.13	A
	ATOM	5020	N	ARG	A	14	6.418	-0.702	33.183	1.00	11.75	A
10	ATOM	5021	CA	ARG	A	14	6.277	0.040	31.939	1.00	11.78	A
	ATOM	5022	CB	ARG	A	14	6.507	-0.912	30.766	1.00	12.75	A
	ATOM	5023	CG	ARG	A	14	7.908	-1.488	30.767	1.00	14.50	A
	ATOM	5024	CD	ARG	A	14	8.186	-2.373	29.566	1.00	15.97	A
	ATOM	5025	NE	ARG	A	14	9.622	-2.433	29.307	1.00	18.20	A
15	ATOM	5026	CZ	ARG	A	14	10.303	-1.488	28.666	1.00	19.33	A
	ATOM	5027	NH1	ARG	A	14	9.678	-0.413	28.202	1.00	19.36	A
	ATOM	5028	NH2	ARG	A	14	11.613	-1.603	28.516	1.00	20.58	A
	ATOM	5029	C	ARG	A	14	4.945	0.753	31.770	1.00	11.74	A
	ATOM	5030	O	ARG	A	14	4.748	1.488	30.801	1.00	11.56	A
20	ATOM	5031	N	ALA	A	15	4.031	0.548	32.709	1.00	11.10	A
	ATOM	5032	CA	ALA	A	15	2.728	1.191	32.618	1.00	10.68	A
	ATOM	5033	CB	ALA	A	15	1.644	0.237	33.111	1.00	10.84	A
	ATOM	5034	C	ALA	A	15	2.665	2.492	33.400	1.00	10.23	A
	ATOM	5035	O	ALA	A	15	1.789	3.322	33.157	1.00	10.48	A
25	ATOM	5036	N	GLU	A	16	3.600	2.679	34.327	1.00	9.72	A

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	ATOM 5037	CA	GLU	A	16	3.618	3.870	35.169	1.00	9.10	A
	ATOM 5038	CB	GLU	A	16	4.808	3.809	36.132	1.00	9.10	A
	ATOM 5039	CG	GLU	A	16	4.692	4.729	37.336	1.00	9.09	A
	ATOM 5040	CD	GLU	A	16	3.527	4.369	38.243	1.00	9.08	A
5	ATOM 5041	OE1	GLU	A	16	2.920	3.291	38.061	1.00	9.56	A
	ATOM 5042	OE2	GLU	A	16	3.218	5.163	39.150	1.00	9.58	A
	ATOM 5043	C	GLU	A	16	3.646	5.194	34.409	1.00	9.31	A
	ATOM 5044	O	GLU	A	16	3.032	6.170	34.837	1.00	8.78	A
	ATOM 5045	N	ILE	A	17	4.361	5.237	33.288	1.00	9.01	A
10	ATOM 5046	CA	ILE	A	17	4.435	6.471	32.517	1.00	8.95	A
	ATOM 5047	CB	ILE	A	17	5.388	6.335	31.303	1.00	9.06	A
	ATOM 5048	CG2	ILE	A	17	4.929	5.211	30.385	1.00	8.42	A
	ATOM 5049	CG1	ILE	A	17	5.449	7.658	30.531	1.00	8.92	A
	ATOM 5050	CD1	ILE	A	17	5.944	8.827	31.354	1.00	9.68	A
15	ATOM 5051	C	ILE	A	17	3.038	6.861	32.044	1.00	9.27	A
	ATOM 5052	O	ILE	A	17	2.701	8.044	31.989	1.00	9.18	A
	ATOM 5242	N	TRP	A	39	-2.568	-14.235	33.625	1.00	32.11	A
	ATOM 5243	CA	TRP	A	39	-1.844	-13.679	32.486	1.00	31.66	A
	ATOM 5244	CB	TRP	A	39	-0.384	-13.406	32.876	1.00	30.89	A
20	ATOM 5245	CG	TRP	A	39	0.496	-12.996	31.726	1.00	30.01	A
	ATOM 5246	CD2	TRP	A	39	0.197	-12.029	30.710	1.00	29.51	A
	ATOM 5247	CE2	TRP	A	39	1.310	-11.981	29.840	1.00	29.33	A
	ATOM 5248	CE3	TRP	A	39	-0.901	-11.197	30.449	1.00	29.25	A
	ATOM 5249	CD1	TRP	A	39	1.741	-13.478	31.440	1.00	29.80	A
25	ATOM 5250	NE1	TRP	A	39	2.237	-12.875	30.308	1.00	29.45	A

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	ATOM 5251	CZ2	TRP	A	39	1.356	-11.136	28.726	1.00	29.02	A
	ATOM 5252	CZ3	TRP	A	39	-0.854	-10.356	29.340	1.00	28.91	A
	ATOM 5253	CH2	TRP	A	39	0.269	-10.333	28.493	1.00	28.96	A
	ATOM 5254	C	TRP	A	39	-1.892	-14.593	31.255	1.00	31.85	A
5	ATOM 5255	O	TRP	A	39	-2.215	-14.142	30.156	1.00	31.82	A
	ATOM 5256	N	PRO	A	40	-1.571	-15.888	31.424	1.00	31.95	A
	ATOM 5257	CD	PRO	A	40	-1.187	-16.569	32.675	1.00	32.13	A
	ATOM 5258	CA	PRO	A	40	-1.586	-16.839	30.306	1.00	32.00	A
	ATOM 5259	CB	PRO	A	40	-1.477	-18.186	31.007	1.00	32.11	A
10	ATOM 5260	CG	PRO	A	40	-0.591	-17.866	32.170	1.00	31.99	A
	ATOM 5261	C	PRO	A	40	-2.830	-16.740	29.427	1.00	31.94	A
	ATOM 5262	O	PRO	A	40	-2.734	-16.751	28.200	1.00	32.11	A
	ATOM 5263	N	GLU	A	41	-3.995	-16.645	30.060	1.00	31.73	A
	ATOM 5264	CA	GLU	A	41	-5.258	-16.542	29.338	1.00	31.51	A
15	ATOM 5265	CB	GLU	A	41	-6.433	-16.620	30.319	1.00	32.22	A
	ATOM 5266	CG	GLU	A	41	-7.807	-16.488	29.668	1.00	33.37	A
	ATOM 5267	CD	GLU	A	41	-8.272	-17.772	29.001	1.00	34.21	A
	ATOM 5268	OE1	GLU	A	41	-7.544	-18.301	28.131	1.00	34.63	A
	ATOM 5269	OE2	GLU	A	41	-9.374	-18.251	29.351	1.00	34.59	A
20	ATOM 5270	C	GLU	A	41	-5.344	-15.236	28.550	1.00	30.86	A
	ATOM 5271	O	GLU	A	41	-5.612	-15.240	27.347	1.00	30.86	A
	ATOM 5272	N	ILE	A	42	-5.116	-14.122	29.239	1.00	29.82	A
	ATOM 5273	CA	ILE	A	42	-5.174	-12.797	28.624	1.00	28.89	A
	ATOM 5274	CB	ILE	A	42	-4.914	-11.697	29.673	1.00	29.12	A
25	ATOM 5275	CG2	ILE	A	42	-4.936	-10.323	29.011	1.00	29.10	A

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	ATOM 5276	CG1	ILE A	42	-5.973	-11.780	30.776	1.00	29.24	A
	ATOM 5277	CD1	ILE A	42	-5.692	-10.894	31.969	1.00	29.54	A
	ATOM 5278	C	ILE A	42	-4.162	-12.637	27.492	1.00	28.04	A
	ATOM 5279	O	ILE A	42	-4.476	-12.078	26.442	1.00	27.96	A
5	ATOM 5280	N	LYS A	43	-2.949	-13.128	27.718	1.00	27.12	A
	ATOM 5281	CA	LYS A	43	-1.877	-13.041	26.733	1.00	26.46	A
	ATOM 5282	CB	LYS A	43	-0.644	-13.791	27.243	1.00	26.21	A
	ATOM 5283	CG	LYS A	43	0.542	-13.791	26.286	1.00	26.04	A
	ATOM 5284	CD	LYS A	43	1.639	-14.723	26.785	1.00	25.92	A
10	ATOM 5285	CE	LYS A	43	2.864	-14.705	25.878	1.00	26.04	A
	ATOM 5286	NZ	LYS A	43	3.565	-13.389	25.888	1.00	25.88	A
	ATOM 5287	C	LYS A	43	-2.282	-13.599	25.371	1.00	26.05	A
	ATOM 5288	O	LYS A	43	-1.989	-13.002	24.333	1.00	25.81	A
	ATOM 5328	N	GLY A	49	0.690	-10.284	22.410	1.00	14.48	A
15	ATOM 5329	CA	GLY A	49	0.907	-10.936	23.690	1.00	14.19	A
	ATOM 5330	C	GLY A	49	1.776	-10.250	24.725	1.00	14.00	A
	ATOM 5331	O	GLY A	49	2.495	-10.913	25.474	1.00	13.78	A
	ATOM 5332	N	LYS A	50	1.702	-8.928	24.792	1.00	13.70	A
	ATOM 5333	CA	LYS A	50	2.505	-8.180	25.749	1.00	13.72	A
20	ATOM 5334	CB	LYS A	50	3.703	-7.544	25.032	1.00	14.43	A
	ATOM 5335	CG	LYS A	50	4.612	-8.550	24.344	1.00	15.06	A
	ATOM 5336	CD	LYS A	50	5.479	-9.277	25.357	1.00	15.66	A
	ATOM 5337	CE	LYS A	50	6.250	-10.411	24.705	1.00	16.36	A
	ATOM 5338	NZ	LYS A	50	6.972	-9.943	23.493	1.00	16.93	A
25	ATOM 5339	C	LYS A	50	1.689	-7.085	26.416	1.00	13.59	A

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	ATOM 5340	O	LYS A	50	0.670	-6.644	25.888	1.00	13.10	A
	ATOM 5341	N	ILE A	51	2.142	-6.661	27.588	1.00	13.34	A
	ATOM 5342	CA	ILE A	51	1.484	-5.588	28.305	1.00	13.51	A
	ATOM 5343	CB	ILE A	51	0.720	-6.100	29.544	1.00	14.11	A
5	ATOM 5344	CG2	ILE A	51	-0.628	-6.656	29.113	1.00	14.02	A
	ATOM 5345	CG1	ILE A	51	1.563	-7.135	30.299	1.00	14.40	A
	ATOM 5346	CD1	ILE A	51	0.909	-7.639	31.571	1.00	15.17	A
	ATOM 5347	C	ILE A	51	2.543	-4.578	28.724	1.00	13.35	A
	ATOM 5348	O	ILE A	51	3.731	-4.892	28.769	1.00	13.56	A
10	ATOM 5349	N	PRO A	52	2.122	-3.355	29.061	1.00	13.08	A
	ATOM 5350	CD	PRO A	52	3.043	-2.244	29.369	1.00	13.17	A
	ATOM 5351	CA	PRO A	52	0.732	-2.892	29.086	1.00	12.94	A
	ATOM 5352	CB	PRO A	52	0.838	-1.561	29.813	1.00	12.82	A
	ATOM 5353	CG	PRO A	52	2.132	-1.022	29.259	1.00	13.02	A
15	ATOM 5354	C	PRO A	52	0.017	-2.716	27.749	1.00	12.81	A
	ATOM 5355	O	PRO A	52	0.625	-2.677	26.677	1.00	12.35	A
	ATOM 5356	N	ILE A	53	-1.300	-2.611	27.846	1.00	12.88	A
	ATOM 5357	CA	ILE A	53	-2.140	-2.343	26.697	1.00	13.33	A
	ATOM 5358	CB	ILE A	53	-2.916	-3.585	26.200	1.00	13.90	A
20	ATOM 5359	CG2	ILE A	53	-1.950	-4.591	25.585	1.00	14.50	A
	ATOM 5360	CG1	ILE A	53	-3.736	-4.186	27.339	1.00	14.62	A
	ATOM 5361	CD1	ILE A	53	-4.703	-5.260	26.878	1.00	15.26	A
	ATOM 5362	C	ILE A	53	-3.132	-1.312	27.213	1.00	13.08	A
	ATOM 5363	O	ILE A	53	-3.373	-1.222	28.421	1.00	13.05	A
25	ATOM 5423	N	HIS A	62	-1.221	-0.970	22.034	1.00	11.06	A

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	ATOM 5424	CA	HIS	A	62	-0.137	-1.598	22.788	1.00	10.38	A
	ATOM 5425	CB	HIS	A	62	0.135	-3.029	22.287	1.00	10.67	A
	ATOM 5426	CG	HIS	A	62	0.735	-3.103	20.917	1.00	11.13	A
	ATOM 5427	CD2	HIS	A	62	1.972	-3.468	20.504	1.00	10.67	A
5	ATOM 5428	ND1	HIS	A	62	0.027	-2.801	19.773	1.00	11.52	A
	ATOM 5429	CE1	HIS	A	62	0.800	-2.978	18.718	1.00	11.13	A
	ATOM 5430	NE2	HIS	A	62	1.987	-3.383	19.134	1.00	12.00	A
	ATOM 5431	C	HIS	A	62	1.136	-0.748	22.707	1.00	9.83	A
	ATOM 5432	O	HIS	A	62	1.162	0.263	22.007	1.00	9.03	A
10	ATOM 5433	N	GLN	A	63	2.169	-1.173	23.436	1.00	9.33	A
	ATOM 5434	CA	GLN	A	63	3.456	-0.486	23.515	1.00	8.74	A
	ATOM 5435	CB	GLN	A	63	4.009	-0.166	22.119	1.00	8.90	A
	ATOM 5436	CG	GLN	A	63	4.690	-1.358	21.414	1.00	8.45	A
	ATOM 5437	CD	GLN	A	63	6.016	-1.771	22.058	1.00	9.03	A
15	ATOM 5438	OE1	GLN	A	63	6.588	-1.032	22.858	1.00	7.87	A
	ATOM 5439	NE2	GLN	A	63	6.513	-2.954	21.691	1.00	8.38	A
	ATOM 5440	C	GLN	A	63	3.316	0.778	24.362	1.00	8.66	A
	ATOM 5441	O	GLN	A	63	2.739	1.783	23.938	1.00	7.74	A
	ATOM 5442	N	SER	A	64	3.855	0.704	25.574	1.00	8.31	A
20	ATOM 5443	CA	SER	A	64	3.766	1.789	26.543	1.00	8.33	A
	ATOM 5444	CB	SER	A	64	4.595	1.446	27.787	1.00	8.01	A
	ATOM 5445	OG	SER	A	64	5.978	1.416	27.493	1.00	7.87	A
	ATOM 5446	C	SER	A	64	4.153	3.172	26.040	1.00	8.36	A
	ATOM 5447	O	SER	A	64	3.435	4.133	26.290	1.00	8.26	A
25	ATOM 5448	N	LEU	A	65	5.274	3.287	25.333	1.00	8.41	A

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	ATOM 5449	CA	LEU	A	65	5.708	4.601	24.866	1.00	8.36	A
	ATOM 5450	CB	LEU	A	65	7.197	4.568	24.514	1.00	8.81	A
	ATOM 5451	CG	LEU	A	65	8.082	4.104	25.687	1.00	9.51	A
	ATOM 5452	CD1	LEU	A	65	9.553	4.275	25.322	1.00	10.70	A
5	ATOM 5453	CD2	LEU	A	65	7.763	4.915	26.941	1.00	9.59	A
	ATOM 5454	C	LEU	A	65	4.867	5.102	23.691	1.00	8.52	A
	ATOM 5455	O	LEU	A	65	4.659	6.308	23.540	1.00	8.38	A
	ATOM 5662	N	ASP	A	93	13.380	7.412	24.678	1.00	8.42	A
	ATOM 5663	CA	ASP	A	93	13.975	6.203	24.118	1.00	9.01	A
10	ATOM 5664	CB	ASP	A	93	14.076	6.291	22.584	1.00	9.85	A
	ATOM 5665	CG	ASP	A	93	12.788	5.838	21.886	1.00	11.05	A
	ATOM 5666	OD1	ASP	A	93	12.750	5.784	20.630	1.00	11.80	A
	ATOM 5667	OD2	ASP	A	93	11.809	5.531	22.605	1.00	11.10	A
	ATOM 5668	C	ASP	A	93	15.344	5.869	24.740	1.00	8.95	A
15	ATOM 5669	O	ASP	A	93	15.656	4.696	24.951	1.00	9.47	A
	ATOM 5670	N	THR	A	94	16.156	6.881	25.036	1.00	8.96	A
	ATOM 5671	CA	THR	A	94	17.462	6.638	25.661	1.00	8.70	A
	ATOM 5672	CB	THR	A	94	18.240	7.965	25.849	1.00	9.08	A
	ATOM 5673	OG1	THR	A	94	18.678	8.430	24.568	1.00	8.81	A
20	ATOM 5674	CG2	THR	A	94	19.462	7.778	26.759	1.00	8.34	A
	ATOM 5675	C	THR	A	94	17.264	5.948	27.017	1.00	9.09	A
	ATOM 5676	O	THR	A	94	17.967	4.987	27.347	1.00	8.99	A
	ATOM 5677	N	LEU	A	95	16.302	6.442	27.792	1.00	8.65	A
	ATOM 5678	CA	LEU	A	95	15.996	5.867	29.094	1.00	9.14	A
25	ATOM 5679	CB	LEU	A	95	14.965	6.725	29.838	1.00	9.16	A

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	ATOM 5680	CG	LEU A	95	15.454	8.091	30.320	1.00	9.32	A
	ATOM 5681	CD1	LEU A	95	14.308	8.874	30.967	1.00	9.37	A
	ATOM 5682	CD2	LEU A	95	16.580	7.876	31.328	1.00	9.77	A
	ATOM 5683	C	LEU A	95	15.462	4.452	28.934	1.00	9.18	A
5	ATOM 5684	O	LEU A	95	15.891	3.539	29.634	1.00	8.68	A
	ATOM 5685	N	ASP A	96	14.529	4.272	28.003	1.00	9.39	A
	ATOM 5686	CA	ASP A	96	13.950	2.960	27.759	1.00	9.93	A
	ATOM 5687	CB	ASP A	96	12.878	3.058	26.668	1.00	11.27	A
	ATOM 5688	CG	ASP A	96	12.035	1.796	26.564	1.00	12.51	A
10	ATOM 5689	OD1	ASP A	96	11.700	1.220	27.616	1.00	14.48	A
	ATOM 5690	OD2	ASP A	96	11.698	1.382	25.444	1.00	13.59	A
	ATOM 5691	C	ASP A	96	15.051	1.981	27.354	1.00	9.66	A
	ATOM 5692	O	ASP A	96	15.094	0.854	27.845	1.00	9.47	A
	ATOM 5693	N	ASP A	97	15.951	2.419	26.476	1.00	9.43	A
15	ATOM 5694	CA	ASP A	97	17.054	1.567	26.034	1.00	9.98	A
	ATOM 5695	CB	ASP A	97	18.033	2.334	25.134	1.00	9.49	A
	ATOM 5696	CG	ASP A	97	17.466	2.650	23.760	1.00	10.73	A
	ATOM 5697	OD1	ASP A	97	18.142	3.390	23.013	1.00	10.05	A
	ATOM 5698	OD2	ASP A	97	16.365	2.164	23.425	1.00	10.69	A
20	ATOM 5699	C	ASP A	97	17.845	1.038	27.230	1.00	10.11	A
	ATOM 5700	O	ASP A	97	18.159	-0.150	27.296	1.00	10.03	A
	ATOM 5701	N	PHE A	98	18.185	1.923	28.164	1.00	10.63	A
	ATOM 5702	CA	PHE A	98	18.965	1.507	29.325	1.00	11.09	A
	ATOM 5703	CB	PHE A	98	19.440	2.717	30.134	1.00	11.78	A
25	ATOM 5704	CG	PHE A	98	20.383	2.358	31.255	1.00	12.44	A

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	ATOM 5705	CD1	PHE	A	98	21.628	1.793	30.983	1.00	12.99	A
	ATOM 5706	CD2	PHE	A	98	20.016	2.555	32.579	1.00	12.82	A
	ATOM 5707	CE1	PHE	A	98	22.494	1.425	32.022	1.00	13.35	A
	ATOM 5708	CE2	PHE	A	98	20.869	2.193	33.623	1.00	13.21	A
5	ATOM 5709	CZ	PHE	A	98	22.109	1.627	33.343	1.00	13.21	A
	ATOM 5710	C	PHE	A	98	18.181	0.565	30.231	1.00	11.33	A
	ATOM 5711	O	PHE	A	98	18.683	-0.494	30.616	1.00	11.57	A
	ATOM 5712	N	MET	A	99	16.951	0.944	30.568	1.00	11.37	A
	ATOM 5713	CA	MET	A	99	16.125	0.113	31.429	1.00	12.06	A
10	ATOM 5714	CB	MET	A	99	14.782	0.796	31.715	1.00	12.55	A
	ATOM 5715	CG	MET	A	99	14.894	2.142	32.413	1.00	13.10	A
	ATOM 5716	SD	MET	A	99	15.806	2.070	33.972	1.00	14.07	A
	ATOM 5717	CE	MET	A	99	14.630	1.211	35.020	1.00	14.27	A
	ATOM 5718	C	MET	A	99	15.877	-1.260	30.812	1.00	12.60	A
15	ATOM 5719	O	MET	A	99	15.754	-2.253	31.528	1.00	12.65	A
	ATOM 5720	N	SER	A	100	15.807	-1.316	29.484	1.00	12.96	A
	ATOM 5721	CA	SER	A	100	15.567	-2.576	28.784	1.00	13.81	A
	ATOM 5722	CB	SER	A	100	15.121	-2.302	27.344	1.00	14.23	A
	ATOM 5723	OG	SER	A	100	13.828	-1.725	27.328	1.00	15.92	A
20	ATOM 5724	C	SER	A	100	16.789	-3.494	28.785	1.00	14.13	A
	ATOM 5725	O	SER	A	100	16.669	-4.686	28.507	1.00	14.04	A
	ATOM 5726	N	CYS	A	101	17.959	-2.938	29.097	1.00	14.67	A
	ATOM 5727	CA	CYS	A	101	19.187	-3.723	29.152	1.00	15.64	A
	ATOM 5728	CB	CYS	A	101	20.415	-2.812	29.235	1.00	16.10	A
25	ATOM 5729	SG	CYS	A	101	20.893	-2.013	27.701	1.00	17.92	A

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	ATOM 5730	C	CYS A 101	19.197	-4.670	30.350	1.00	15.85	A
	ATOM 5731	O	CYS A 101	19.926	-5.662	30.350	1.00	15.88	A
	ATOM 5732	N	PHE A 102	18.404	-4.361	31.373	1.00	15.73	A
	ATOM 5733	CA	PHE A 102	18.343	-5.214	32.562	1.00	15.76	A
5	ATOM 5734	CB	PHE A 102	17.748	-4.462	33.754	1.00	15.27	A
	ATOM 5735	CG	PHE A 102	18.613	-3.348	34.258	1.00	15.10	A
	ATOM 5736	CD1	PHE A 102	18.642	-2.125	33.600	1.00	14.99	A
	ATOM 5737	CD2	PHE A 102	19.414	-3.527	35.380	1.00	14.73	A
	ATOM 5738	CE1	PHE A 102	19.457	-1.092	34.050	1.00	15.09	A
10	ATOM 5739	CE2	PHE A 102	20.237	-2.500	35.841	1.00	14.94	A
	ATOM 5740	CZ	PHE A 102	20.256	-1.280	35.174	1.00	14.83	A
	ATOM 5741	C	PHE A 102	17.505	-6.455	32.295	1.00	16.19	A
	ATOM 5742	O	PHE A 102	16.415	-6.366	31.728	1.00	15.63	A
	ATOM 5743	N	PRO A 103	18.009	-7.632	32.699	1.00	16.76	A
15	ATOM 5744	CD	PRO A 103	19.356	-7.845	33.260	1.00	17.02	A
	ATOM 5745	CA	PRO A 103	17.319	-8.914	32.512	1.00	17.47	A
	ATOM 5746	CB	PRO A 103	18.456	-9.923	32.609	1.00	17.20	A
	ATOM 5747	CG	PRO A 103	19.315	-9.315	33.668	1.00	17.07	A
	ATOM 5748	C	PRO A 103	16.246	-9.145	33.577	1.00	18.16	A
20	ATOM 5749	O	PRO A 103	16.363	-10.043	34.418	1.00	18.22	A
	ATOM 5750	N	TRP A 104	15.197	-8.331	33.525	1.00	18.78	A
	ATOM 5751	CA	TRP A 104	14.099	-8.414	34.482	1.00	19.84	A
	ATOM 5752	CB	TRP A 104	13.017	-7.381	34.141	1.00	18.95	A
	ATOM 5753	CG	TRP A 104	13.517	-5.971	34.076	1.00	18.24	A
25	ATOM 5754	CD2	TRP A 104	13.896	-5.144	35.182	1.00	17.79	A

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	ATOM 5755	CE2 TRP A 104	14.321	-3.906	34.652	1.00	17.69	A
	ATOM 5756	CE3 TRP A 104	13.921	-5.329	36.572	1.00	17.54	A
	ATOM 5757	CD1 TRP A 104	13.720	-5.224	32.951	1.00	17.72	A
	ATOM 5758	NE1 TRP A 104	14.201	-3.981	33.289	1.00	17.64	A
5	ATOM 5759	CZ2 TRP A 104	14.765	-2.856	35.463	1.00	17.79	A
	ATOM 5760	CZ3 TRP A 104	14.363	-4.282	37.379	1.00	17.58	A
	ATOM 5761	CH2 TRP A 104	14.778	-3.064	36.820	1.00	17.48	A
	ATOM 5762	C TRP A 104	13.449	-9.790	34.572	1.00	20.99	A
	ATOM 5763	O TRP A 104	13.031	-10.207	35.650	1.00	21.33	A
10	ATOM 5764	N ALA A 105	13.359	-10.493	33.447	1.00	22.46	A
	ATOM 5765	CA ALA A 105	12.720	-11.807	33.434	1.00	23.88	A
	ATOM 5766	CB ALA A 105	11.878	-11.961	32.169	1.00	23.69	A
	ATOM 5767	C ALA A 105	13.685	-12.982	33.565	1.00	24.90	A
	ATOM 5768	O ALA A 105	13.262	-14.136	33.576	1.00	25.13	A
15	ATOM 5769	N GLU A 106	14.976	-12.686	33.675	1.00	26.10	A
	ATOM 5770	CA GLU A 106	15.996	-13.721	33.803	1.00	27.43	A
	ATOM 5771	CB GLU A 106	17.388	-13.083	33.790	1.00	27.61	A
	ATOM 5772	CG GLU A 106	18.550	-14.065	33.842	1.00	28.16	A
	ATOM 5773	CD GLU A 106	18.455	-15.144	32.775	1.00	28.35	A
20	ATOM 5774	OE1 GLU A 106	17.850	-16.200	33.045	1.00	28.68	A
	ATOM 5775	OE2 GLU A 106	18.973	-14.931	31.662	1.00	28.90	A
	ATOM 5776	C GLU A 106	15.823	-14.543	35.077	1.00	28.31	A
	ATOM 5777	O GLU A 106	15.898	-14.010	36.185	1.00	28.41	A
	ATOM 5778	N LYS A 107	15.591	-15.842	34.908	1.00	29.48	A
25	ATOM 5779	CA LYS A 107	15.420	-16.754	36.038	1.00	30.63	A

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	ATOM 5780	CB	LYS A 107	14.695	-18.028	35.594	1.00	31.06	A
	ATOM 5781	CG	LYS A 107	13.187	-18.016	35.779	1.00	31.97	A
	ATOM 5782	CD	LYS A 107	12.495	-17.030	34.864	1.00	32.92	A
	ATOM 5783	CE	LYS A 107	10.983	-17.201	34.945	1.00	33.65	A
5	ATOM 5784	NZ	LYS A 107	10.485	-17.067	36.346	1.00	34.05	A
	ATOM 5785	C	LYS A 107	16.775	-17.133	36.630	1.00	31.06	A
	ATOM 5786	O	LYS A 107	16.874	-17.465	37.810	1.00	31.19	A
	ATOM 5787	N	LYS A 108	17.810	-17.094	35.796	1.00	31.69	A
	ATOM 5788	CA	LYS A 108	19.163	-17.421	36.231	1.00	32.35	A
10	ATOM 5789	CB	LYS A 108	20.082	-17.563	35.017	1.00	32.50	A
	ATOM 5790	CG	LYS A 108	19.634	-18.632	34.033	1.00	32.81	A
	ATOM 5791	CD	LYS A 108	20.454	-18.602	32.757	1.00	33.35	A
	ATOM 5792	CE	LYS A 108	19.977	-19.664	31.777	1.00	33.34	A
	ATOM 5793	NZ	LYS A 108	20.660	-19.552	30.454	1.00	33.69	A
15	ATOM 5794	C	LYS A 108	19.668	-16.305	37.143	1.00	32.68	A
	ATOM 5795	O	LYS A 108	20.180	-15.288	36.675	1.00	32.69	A
	ATOM 5796	N	GLN A 109	19.518	-16.510	38.447	1.00	33.05	A
	ATOM 5797	CA	GLN A 109	19.923	-15.529	39.443	1.00	33.40	A
	ATOM 5798	CB	GLN A 109	19.719	-16.101	40.846	1.00	34.05	A
20	ATOM 5799	CG	GLN A 109	18.943	-15.175	41.763	1.00	34.95	A
	ATOM 5800	CD	GLN A 109	17.561	-14.854	41.223	1.00	35.27	A
	ATOM 5801	OE1	GLN A 109	16.934	-13.878	41.633	1.00	35.73	A
	ATOM 5802	NE2	GLN A 109	17.077	-15.682	40.301	1.00	35.62	A
	ATOM 5803	C	GLN A 109	21.360	-15.042	39.293	1.00	33.21	A
25	ATOM 5804	O	GLN A 109	21.619	-13.842	39.374	1.00	33.28	A

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	ATOM 5805	N	ASP A 110	22.290	-15.966	39.078	1.00	32.78	A
	ATOM 5806	CA	ASP A 110	23.692	-15.597	38.927	1.00	32.30	A
	ATOM 5807	CB	ASP A 110	24.569	-16.852	38.841	1.00	32.93	A
	ATOM 5808	CG	ASP A 110	24.303	-17.670	37.592	1.00	33.42	A
5	ATOM 5809	OD1	ASP A 110	23.137	-18.065	37.371	1.00	33.92	A
	ATOM 5810	OD2	ASP A 110	25.263	-17.921	36.832	1.00	33.95	A
	ATOM 5811	C	ASP A 110	23.891	-14.734	37.684	1.00	31.55	A
	ATOM 5812	O	ASP A 110	24.641	-13.759	37.708	1.00	31.47	A
	ATOM 5813	N	VAL A 111	23.211	-15.096	36.600	1.00	30.50	A
10	ATOM 5814	CA	VAL A 111	23.310	-14.352	35.350	1.00	29.55	A
	ATOM 5815	CB	VAL A 111	22.661	-15.130	34.188	1.00	29.61	A
	ATOM 5816	CG1	VAL A 111	22.743	-14.322	32.907	1.00	29.78	A
	ATOM 5817	CG2	VAL A 111	23.353	-16.469	34.017	1.00	29.84	A
	ATOM 5818	C	VAL A 111	22.613	-13.000	35.485	1.00	28.61	A
15	ATOM 5819	O	VAL A 111	23.069	-11.995	34.939	1.00	28.38	A
	ATOM 5820	N	LYS A 112	21.509	-12.986	36.224	1.00	27.55	A
	ATOM 5821	CA	LYS A 112	20.746	-11.763	36.435	1.00	26.48	A
	ATOM 5822	CB	LYS A 112	19.414	-12.083	37.117	1.00	26.47	A
	ATOM 5823	CG	LYS A 112	18.452	-10.907	37.177	1.00	25.94	A
20	ATOM 5824	CD	LYS A 112	17.173	-11.278	37.904	1.00	26.05	A
	ATOM 5825	CE	LYS A 112	16.181	-10.125	37.906	1.00	25.77	A
	ATOM 5826	NZ	LYS A 112	14.951	-10.457	38.676	1.00	25.64	A
	ATOM 5827	C	LYS A 112	21.523	-10.765	37.287	1.00	26.12	A
	ATOM 5828	O	LYS A 112	21.631	-9.589	36.941	1.00	25.60	A
25	ATOM 5829	N	GLU A 113	22.062	-11.243	38.404	1.00	25.24	A

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	ATOM 5830	CA	GLU A 113	22.818	-10.393	39.314	1.00	25.10	A
	ATOM 5831	CB	GLU A 113	23.128	-11.159	40.605	1.00	25.39	A
	ATOM 5832	CG	GLU A 113	23.862	-10.347	41.669	1.00	25.63	A
	ATOM 5833	CD	GLU A 113	23.026	-9.213	42.248	1.00	25.83	A
5	ATOM 5834	OE1	GLU A 113	23.522	-8.525	43.170	1.00	25.56	A
	ATOM 5835	OE2	GLU A 113	21.880	-9.008	41.786	1.00	25.58	A
	ATOM 5836	C	GLU A 113	24.113	-9.891	38.676	1.00	24.67	A
	ATOM 5837	O	GLU A 113	24.578	-8.791	38.975	1.00	24.33	A
	ATOM 5838	N	GLN A 114	24.689	-10.702	37.796	1.00	24.42	A
10	ATOM 5839	CA	GLN A 114	25.926	-10.341	37.116	1.00	24.24	A
	ATOM 5840	CB	GLN A 114	26.438	-11.538	36.308	1.00	24.91	A
	ATOM 5841	CG	GLN A 114	27.868	-11.417	35.789	1.00	25.97	A
	ATOM 5842	CD	GLN A 114	28.030	-10.372	34.700	1.00	26.74	A
	ATOM 5843	OE1	GLN A 114	27.278	-10.353	33.723	1.00	26.88	A
15	ATOM 5844	NE2	GLN A 114	29.026	-9.502	34.856	1.00	27.12	A
	ATOM 5845	C	GLN A 114	25.685	-9.148	36.193	1.00	23.68	A
	ATOM 5846	O	GLN A 114	26.465	-8.194	36.180	1.00	23.45	A
	ATOM 5847	N	MET A 115	24.598	-9.196	35.429	1.00	22.98	A
	ATOM 5848	CA	MET A 115	24.284	-8.113	34.503	1.00	22.57	A
20	ATOM 5849	CB	MET A 115	23.229	-8.566	33.489	1.00	24.00	A
	ATOM 5850	CG	MET A 115	22.980	-7.560	32.371	1.00	25.61	A
	ATOM 5851	SD	MET A 115	24.507	-6.939	31.592	1.00	28.29	A
	ATOM 5852	CE	MET A 115	24.966	-8.333	30.583	1.00	27.44	A
	ATOM 5853	C	MET A 115	23.815	-6.855	35.228	1.00	21.47	A
25	ATOM 5854	O	MET A 115	24.191	-5.747	34.851	1.00	20.89	A

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	ATOM 5855	N	PHE A 116	22.998	-7.025	36.265	1.00	20.55	A
	ATOM 5856	CA	PHE A 116	22.515	-5.882	37.033	1.00	19.83	A
	ATOM 5857	CB	PHE A 116	21.626	-6.334	38.195	1.00	19.24	A
	ATOM 5858	CG	PHE A 116	20.154	-6.260	37.901	1.00	18.22	A
5	ATOM 5859	CD1	PHE A 116	19.554	-7.163	37.030	1.00	17.96	A
	ATOM 5860	CD2	PHE A 116	19.368	-5.284	38.501	1.00	17.91	A
	ATOM 5861	CE1	PHE A 116	18.186	-7.096	36.761	1.00	17.74	A
	ATOM 5862	CE2	PHE A 116	18.001	-5.205	38.241	1.00	17.75	A
	ATOM 5863	CZ	PHE A 116	17.409	-6.114	37.368	1.00	17.62	A
10	ATOM 5864	C	PHE A 116	23.701	-5.110	37.593	1.00	20.07	A
	ATOM 5865	O	PHE A 116	23.789	-3.891	37.450	1.00	19.59	A
	ATOM 6152	N	TYR A 152	9.211	10.332	32.716	1.00	8.70	A
	ATOM 6153	CA	TYR A 152	9.897	9.070	32.511	1.00	8.91	A
	ATOM 6154	CB	TYR A 152	10.120	8.824	31.021	1.00	9.31	A
15	ATOM 6155	CG	TYR A 152	10.158	7.355	30.660	1.00	10.11	A
	ATOM 6156	CD1	TYR A 152	9.197	6.466	31.160	1.00	10.35	A
	ATOM 6157	CE1	TYR A 152	9.215	5.109	30.811	1.00	10.49	A
	ATOM 6158	CD2	TYR A 152	11.137	6.854	29.804	1.00	10.28	A
	ATOM 6159	CE2	TYR A 152	11.160	5.505	29.448	1.00	10.37	A
20	ATOM 6160	CZ	TYR A 152	10.206	4.642	29.950	1.00	10.60	A
	ATOM 6161	OH	TYR A 152	10.245	3.314	29.587	1.00	10.57	A
	ATOM 6162	C	TYR A 152	11.211	9.033	33.272	1.00	9.20	A
	ATOM 6163	O	TYR A 152	11.622	7.982	33.759	1.00	9.19	A
	ATOM 6164	N	TRP A 153	11.869	10.180	33.386	1.00	9.22	A
25	ATOM 6165	CA	TRP A 153	13.113	10.224	34.135	1.00	9.64	A

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	ATOM 6166	CB	TRP	A	153	13.752	11.613	34.067	1.00	10.03	A
	ATOM 6167	CG	TRP	A	153	14.748	11.836	35.157	1.00	10.79	A
	ATOM 6168	CD2	TRP	A	153	15.900	11.033	35.441	1.00	11.30	A
	ATOM 6169	CE2	TRP	A	153	16.521	11.583	36.585	1.00	11.43	A
5	ATOM 6170	CE3	TRP	A	153	16.467	9.899	34.841	1.00	11.63	A
	ATOM 6171	CD1	TRP	A	153	14.717	12.816	36.111	1.00	10.88	A
	ATOM 6172	NE1	TRP	A	153	15.780	12.669	36.974	1.00	11.27	A
	ATOM 6173	CZ2	TRP	A	153	17.682	11.040	37.142	1.00	11.66	A
	ATOM 6174	CZ3	TRP	A	153	17.629	9.354	35.398	1.00	12.00	A
10	ATOM 6175	CH2	TRP	A	153	18.221	9.931	36.539	1.00	11.19	A
	ATOM 6176	C	TRP	A	153	12.836	9.867	35.593	1.00	9.64	A
	ATOM 6177	O	TRP	A	153	13.518	9.022	36.175	1.00	9.85	A
	ATOM 6178	N	GLU	A	154	11.827	10.504	36.177	1.00	9.88	A
	ATOM 6179	CA	GLU	A	154	11.491	10.260	37.570	1.00	9.73	A
15	ATOM 6180	CB	GLU	A	154	10.379	11.222	38.007	1.00	10.24	A
	ATOM 6181	CG	GLU	A	154	10.187	11.310	39.509	1.00	11.28	A
	ATOM 6182	CD	GLU	A	154	9.315	10.199	40.035	1.00	11.50	A
	ATOM 6183	OE1	GLU	A	154	9.291	9.987	41.267	1.00	12.33	A
	ATOM 6184	OE2	GLU	A	154	8.645	9.543	39.207	1.00	12.17	A
20	ATOM 6185	C	GLU	A	154	11.081	8.802	37.785	1.00	9.53	A
	ATOM 6186	O	GLU	A	154	11.468	8.180	38.776	1.00	9.12	A
	ATOM 6187	N	ILE	A	155	10.320	8.257	36.837	1.00	8.98	A
	ATOM 6188	CA	ILE	A	155	9.870	6.875	36.904	1.00	8.87	A
	ATOM 6189	CB	ILE	A	155	8.810	6.599	35.815	1.00	8.72	A
25	ATOM 6190	CG2	ILE	A	155	8.550	5.097	35.683	1.00	9.06	A

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	ATOM 6191	CG1	ILE A 155	7.524	7.354	36.173	1.00	8.74	A
	ATOM 6192	CD1	ILE A 155	6.467	7.383	35.064	1.00	8.73	A
	ATOM 6193	C	ILE A 155	11.035	5.888	36.782	1.00	9.35	A
	ATOM 6194	O	ILE A 155	11.180	4.986	37.609	1.00	9.36	A
5	ATOM 6195	N	CYS A 156	11.873	6.063	35.766	1.00	9.31	A
	ATOM 6196	CA	CYS A 156	13.012	5.175	35.589	1.00	10.15	A
	ATOM 6197	CB	CYS A 156	13.734	5.471	34.269	1.00	10.37	A
	ATOM 6198	SG	CYS A 156	12.770	5.037	32.774	1.00	11.81	A
	ATOM 6199	C	CYS A 156	14.008	5.280	36.741	1.00	10.50	A
10	ATOM 6200	O	CYS A 156	14.480	4.262	37.247	1.00	10.92	A
	ATOM 6201	N	SER A 157	14.325	6.499	37.163	1.00	10.75	A
	ATOM 6202	CA	SER A 157	15.291	6.680	38.246	1.00	10.88	A
	ATOM 6203	CB	SER A 157	15.633	8.167	38.431	1.00	11.09	A
	ATOM 6204	OG	SER A 157	14.501	8.948	38.749	1.00	11.29	A
15	ATOM 6205	C	SER A 157	14.813	6.073	39.565	1.00	11.31	A
	ATOM 6206	O	SER A 157	15.618	5.576	40.357	1.00	11.45	A
	ATOM 6207	N	THR A 158	13.506	6.113	39.799	1.00	11.14	A
	ATOM 6208	CA	THR A 158	12.932	5.538	41.008	1.00	11.46	A
	ATOM 6209	CB	THR A 158	11.396	5.654	40.996	1.00	10.96	A
20	ATOM 6210	OG1	THR A 158	11.028	7.026	41.168	1.00	11.35	A
	ATOM 6211	CG2	THR A 158	10.775	4.806	42.114	1.00	10.93	A
	ATOM 6212	C	THR A 158	13.310	4.059	41.104	1.00	11.75	A
	ATOM 6213	O	THR A 158	13.749	3.588	42.151	1.00	11.75	A
	ATOM 6214	N	THR A 159	13.139	3.328	40.006	1.00	11.91	A
25	ATOM 6215	CA	THR A 159	13.470	1.910	40.002	1.00	12.52	A

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	ATOM 6216	CB	THR	A	159	12.884	1.205	38.760	1.00	12.63	A
	ATOM 6217	OG1	THR	A	159	11.455	1.252	38.832	1.00	12.91	A
	ATOM 6218	CG2	THR	A	159	13.327	-0.263	38.705	1.00	12.73	A
	ATOM 6219	C	THR	A	159	14.978	1.666	40.084	1.00	12.45	A
5	ATOM 6220	O	THR	A	159	15.424	0.723	40.739	1.00	12.48	A
	ATOM 6221	N	LEU	A	160	15.767	2.516	39.436	1.00	12.52	A
	ATOM 6222	CA	LEU	A	160	17.215	2.356	39.490	1.00	12.72	A
	ATOM 6223	CB	LEU	A	160	17.908	3.355	38.555	1.00	12.33	A
	ATOM 6224	CG	LEU	A	160	17.690	3.148	37.047	1.00	13.04	A
10	ATOM 6225	CD1	LEU	A	160	18.367	4.267	36.268	1.00	12.38	A
	ATOM 6226	CD2	LEU	A	160	18.247	1.793	36.629	1.00	12.53	A
	ATOM 6227	C	LEU	A	160	17.716	2.563	40.922	1.00	12.87	A
	ATOM 6228	O	LEU	A	160	18.607	1.850	41.380	1.00	13.07	A
	ATOM 6229	N	LEU	A	161	17.130	3.528	41.628	1.00	13.22	A
15	ATOM 6230	CA	LEU	A	161	17.530	3.828	43.000	1.00	13.77	A
	ATOM 6231	CB	LEU	A	161	16.833	5.102	43.490	1.00	13.77	A
	ATOM 6232	CG	LEU	A	161	17.314	6.417	42.863	1.00	13.80	A
	ATOM 6233	CD1	LEU	A	161	16.371	7.552	43.241	1.00	13.46	A
	ATOM 6234	CD2	LEU	A	161	18.736	6.723	43.329	1.00	13.49	A
20	ATOM 6235	C	LEU	A	161	17.252	2.684	43.967	1.00	14.34	A
	ATOM 6236	O	LEU	A	161	17.839	2.619	45.050	1.00	14.37	A
	ATOM 6237	N	VAL	A	162	16.350	1.792	43.578	1.00	14.42	A
	ATOM 6238	CA	VAL	A	162	16.019	0.639	44.404	1.00	15.39	A
	ATOM 6239	CB	VAL	A	162	14.826	-0.146	43.813	1.00	15.43	A
25	ATOM 6240	CG1	VAL	A	162	14.643	-1.467	44.565	1.00	15.56	A

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	ATOM 6241	CG2	VAL	A	162	13.559	0.698	43.910	1.00	15.37	A
	ATOM 6242	C	VAL	A	162	17.232	-0.289	44.493	1.00	16.01	A
	ATOM 6243	O	VAL	A	162	17.490	-0.899	45.535	1.00	16.21	A
	ATOM 6244	N	PHE	A	163	17.982	-0.381	43.399	1.00	16.34	A
5	ATOM 6245	CA	PHE	A	163	19.160	-1.237	43.354	1.00	17.20	A
	ATOM 6246	CB	PHE	A	163	19.218	-1.999	42.026	1.00	17.31	A
	ATOM 6247	CG	PHE	A	163	17.979	-2.791	41.729	1.00	18.00	A
	ATOM 6248	CD1	PHE	A	163	16.865	-2.177	41.173	1.00	18.03	A
	ATOM 6249	CD2	PHE	A	163	17.917	-4.149	42.029	1.00	18.06	A
10	ATOM 6250	CE1	PHE	A	163	15.704	-2.900	40.922	1.00	18.23	A
	ATOM 6251	CE2	PHE	A	163	16.757	-4.884	41.782	1.00	18.01	A
	ATOM 6252	CZ	PHE	A	163	15.649	-4.258	41.227	1.00	18.18	A
	ATOM 6253	C	PHE	A	163	20.470	-0.482	43.553	1.00	17.48	A
	ATOM 6254	O	PHE	A	163	21.473	-1.078	43.937	1.00	17.90	A
15	ATOM 6528	N	THR	A	197	4.591	-0.941	45.453	1.00	17.89	A
	ATOM 6529	CA	THR	A	197	5.221	-2.157	44.953	1.00	17.58	A
	ATOM 6530	CB	THR	A	197	4.623	-2.571	43.592	1.00	17.29	A
	ATOM 6531	OG1	THR	A	197	4.796	-1.501	42.652	1.00	17.06	A
	ATOM 6532	CG2	THR	A	197	3.135	-2.881	43.732	1.00	17.03	A
20	ATOM 6533	C	THR	A	197	6.712	-1.903	44.780	1.00	17.29	A
	ATOM 6534	O	THR	A	197	7.139	-0.757	44.661	1.00	17.19	A
	ATOM 6535	N	LYS	A	198	7.507	-2.967	44.775	1.00	17.12	A
	ATOM 6536	CA	LYS	A	198	8.948	-2.813	44.620	1.00	17.28	A
	ATOM 6537	CB	LYS	A	198	9.647	-4.168	44.727	1.00	17.40	A
25	ATOM 6538	CG	LYS	A	198	11.159	-4.088	44.582	1.00	17.55	A

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	ATOM 6539	CD	LYS A 198	11.792	-5.459	44.688	1.00	17.80	A
	ATOM 6540	CE	LYS A 198	13.304	-5.355	44.747	1.00	17.96	A
	ATOM 6541	NZ	LYS A 198	13.944	-6.692	44.918	1.00	19.01	A
	ATOM 6542	C	LYS A 198	9.292	-2.172	43.280	1.00	17.06	A
5	ATOM 6543	O	LYS A 198	9.996	-1.163	43.225	1.00	16.95	A
	ATOM 6544	N	LEU A 199	8.783	-2.762	42.205	1.00	17.25	A
	ATOM 6545	CA	LEU A 199	9.049	-2.271	40.860	1.00	17.51	A
	ATOM 6546	CB	LEU A 199	9.557	-3.420	39.987	1.00	18.10	A
	ATOM 6547	CG	LEU A 199	10.722	-4.239	40.550	1.00	18.31	A
10	ATOM 6548	CD1	LEU A 199	11.046	-5.365	39.591	1.00	18.98	A
	ATOM 6549	CD2	LEU A 199	11.941	-3.350	40.768	1.00	18.60	A
	ATOM 6550	C	LEU A 199	7.804	-1.655	40.228	1.00	17.54	A
	ATOM 6551	O	LEU A 199	6.789	-1.503	40.943	1.00	17.46	A
	ATOM 6552	OXT	LEU A 199	7.864	-1.331	39.025	1.00	17.38	A
15	ATOM 6613	N1	GSH H 200	8.267	-2.783	25.084	1.00	18.14	H
	ATOM 6614	CA1	GSH H 200	6.892	-3.012	25.512	1.00	18.05	H
	ATOM 6615	C1	GSH H 200	6.253	-1.716	26.049	1.00	17.74	H
	ATOM 6616	O11	GSH H 200	6.974	-0.743	26.300	1.00	17.76	H
	ATOM 6617	O12	GSH H 200	4.957	-1.770	26.305	1.00	17.69	H
20	ATOM 6618	CB1	GSH H 200	6.915	-4.033	26.658	1.00	18.51	H
	ATOM 6619	CG1	GSH H 200	6.911	-5.492	26.184	1.00	19.29	H
	ATOM 6620	CD1	GSH H 200	7.126	-6.355	27.445	1.00	18.72	H
	ATOM 6621	OE1	GSH H 200	8.184	-6.947	27.593	1.00	19.64	H
	ATOM 6622	N2	GSH H 200	6.110	-6.407	28.322	1.00	18.69	H
25	ATOM 6623	CA2	GSH H 200	6.216	-7.299	29.489	1.00	18.57	H

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	ATOM 6624	C2	GSH H 200	5.273	-8.489	29.291	1.00	19.14	H
	ATOM 6625	O2	GSH H 200	4.151	-8.358	28.784	1.00	19.07	H
	ATOM 6626	CB2	GSH H 200	5.800	-6.596	30.799	1.00	18.29	H
	ATOM 6627	SG2	GSH H 200	7.094	-5.503	31.467	1.00	17.57	H
5	ATOM 6628	N3	GSH H 200	5.713	-9.677	29.767	1.00	19.66	H
	ATOM 6629	CA3	GSH H 200	4.866	-10.887	29.805	1.00	20.05	H
	ATOM 6630	C3	GSH H 200	5.256	-11.824	28.677	1.00	20.59	H
	ATOM 6631	O31	GSH H 200	4.643	-12.911	28.623	1.00	20.61	H
	ATOM 6632	O32	GSH H 200	6.164	-11.461	27.881	1.00	20.69	H
10	ATOM 6633	CA+2 CA2	M 900	12.319	1.399	22.690	1.00	23.39	M
	ATOM 6700	OH2	WAT S 68	14.121	2.911	22.047	1.00	14.43	S
	ATOM 6701	OH2	WAT S 69	10.382	0.015	22.374	1.00	17.83	S
	ATOM 6702	OH2	WAT S 70	6.835	1.587	23.510	1.00	10.00	S
	ATOM 6703	OH2	WAT S 71	9.084	0.596	24.637	1.00	20.95	S
15	ATOM 6704	OH2	WAT S 72	7.464	2.364	29.866	1.00	18.58	S
	ATOM 6705	OH2	WAT S 73	6.627	3.292	32.747	1.00	10.51	S
	ATOM 6706	OH2	WAT S 74	10.027	-0.425	37.514	1.00	16.92	S
	ATOM 6707	OH2	WAT S 75	8.932	1.748	36.205	1.00	14.34	S
	ATOM 6708	OH2	WAT S 76	9.214	3.513	38.532	1.00	18.39	S
20	ATOM 6736	OH2	WAT S 106	8.886	-7.534	20.205	1.00	13.51	S
	ATOM 6737	OH2	WAT S 107	3.110	-4.937	22.720	1.00	12.05	S
	ATOM 6738	OH2	WAT S 108	0.868	-6.588	23.134	1.00	10.94	S
	ATOM 6739	OH2	WAT S 109	5.765	-8.770	20.668	1.00	22.48	S
	ATOM 6740	OH2	WAT S 110	7.826	-6.141	22.398	1.00	11.14	S
25	ATOM 6741	OH2	WAT S 111	5.382	-6.173	21.467	1.00	10.04	S

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	ATOM 6742	OH2 WAT S 112	13.216	-1.032	21.636	1.00	18.10	S
	ATOM 6744	OH2 WAT S 114	17.856	-1.808	25.058	1.00	20.41	S
	ATOM 6760	OH2 WAT S 130	3.197	-14.232	20.833	1.00	51.90	S
	ATOM 6991	OH2 WAT S 374	1.473	2.207	40.356	1.00	10.67	S
5	ATOM 6992	OH2 WAT S 375	4.951	1.805	44.037	1.00	15.41	S
	ATOM 7014	OH2 WAT S 399	-1.260	-6.795	21.531	1.00	15.82	S
	ATOM 7015	OH2 WAT S 400	-2.774	-4.748	20.376	1.00	27.99	S
	ATOM 7018	OH2 WAT S 403	2.577	0.177	41.980	1.00	13.62	S
	ATOM 7019	OH2 WAT S 404	0.564	-8.538	39.036	1.00	23.05	S
10	ATOM 7020	OH2 WAT S 405	8.238	-9.999	31.265	1.00	29.66	S
	ATOM 7040	OH2 WAT S 426	11.203	0.001	32.951	1.00	36.44	S
	ATOM 7041	OH2 WAT S 428	15.066	-17.180	32.416	1.00	31.37	S
	ATOM 7042	OH2 WAT S 429	10.965	-7.436	30.782	1.00	46.48	S
	ATOM 7053	OH2 WAT S 443	-2.454	-1.326	35.257	1.00	9.90	S
15	ATOM 7075	OH2 WAT S 476	9.258	-15.961	22.392	1.00	35.74	S
	ATOM 7079	OH2 WAT S 484	18.667	-6.199	25.509	1.00	51.86	S
	ATOM 7181	OH2 WAT S 609	14.259	0.633	24.144	1.00	13.45	S
	ATOM 7185	OH2 WAT S 616	6.184	-5.556	45.296	1.00	23.90	S
	ATOM 7186	OH2 WAT S 617	8.234	-7.048	46.247	1.00	26.45	S
20	ATOM 7201	OH2 WAT S 637	8.943	-7.562	24.594	1.00	21.20	S
	ATOM 7202	OH2 WAT S 638	10.718	-9.017	21.394	1.00	20.69	S
	ATOM 7203	OH2 WAT S 639	6.772	-12.758	20.621	1.00	31.01	S
	ATOM 7204	OH2 WAT S 640	4.298	-12.631	22.679	1.00	44.61	S
	ATOM 7205	OH2 WAT S 642	11.438	-5.078	25.419	1.00	41.38	S
25	ATOM 7215	OH2 WAT S 657	2.956	-3.352	25.272	1.00	13.15	S

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	ATOM	7232	OH2 WAT S	690	14.369	-9.780	30.964	1.00	44.36	S
	ATOM	7233	OH2 WAT S	692	18.178	-7.756	40.325	1.00	19.70	S
	ATOM	7235	OH2 WAT S	696	7.112	-5.132	42.047	1.00	21.00	S
	ATOM	7237	OH2 WAT S	698	8.595	-7.307	41.589	1.00	30.04	S
5	ATOM	7238	OH2 WAT S	699	13.321	-7.321	42.140	1.00	27.80	S
	ATOM	7240	OH2 WAT S	702	-6.903	-2.845	28.812	1.00	20.55	S
	ATOM	7245	OH2 WAT S	707	10.773	3.112	22.561	1.00	18.01	S
	ATOM	7249	OH2 WAT S	713	14.133	-12.827	37.720	1.00	37.72	S
	ATOM	7257	OH2 WAT S	729	9.660	-4.357	34.020	1.00	40.28	S
10	ATOM	7260	OH2 WAT S	735	10.625	-2.519	35.392	1.00	46.30	S
	ATOM	7291	OH2 WAT S	783	8.130	-9.654	27.367	1.00	21.27	S
	ATOM	7318	OH2 WAT S	831	5.332	-11.112	19.145	1.00	24.71	S
	ATOM	7333	OH2 WAT S	860	15.591	-0.692	20.940	1.00	38.98	S
	ATOM	7334	OH2 WAT S	861	15.057	-5.068	23.204	1.00	45.10	S
15	ATOM	7336	OH2 WAT S	864	17.064	-8.176	25.940	1.00	41.30	S
	ATOM	7368	OH2 WAT S	916	4.717	-6.156	42.468	1.00	32.94	S
	ATOM	7371	OH2 WAT S	920	19.610	-12.642	30.175	1.00	31.99	S
	ATOM	7386	OH2 WAT S	948	12.372	1.268	20.616	1.00	22.94	S
	ATOM	7399	OH2 WAT S	968	7.575	-13.636	26.467	1.00	40.77	S
20	ATOM	7400	OH2 WAT S	969	13.034	-12.270	21.957	1.00	29.54	S
	ATOM	7415	OH2 WAT T	1	13.128	-8.340	38.325	1.00	43.19	T
	ATOM	7416	OH2 WAT T	2	9.607	-8.619	44.219	1.00	27.56	T
	ATOM	7503	OH2 WAT T	98	3.711	-6.417	45.304	1.00	30.04	T
	ATOM	7507	OH2 WAT T	102	-3.417	-7.320	40.850	1.00	33.06	T
25	ATOM	7602	OH2 WAT T	203	14.604	-1.609	23.500	1.00	40.59	T

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	ATOM 7612	OH2	WAT	T	215	4.850	-13.737	39.498	1.00	42.03	T
	ATOM 7613	OH2	WAT	T	216	5.093	-14.055	32.065	1.00	39.20	T
	ATOM 7616	OH2	WAT	T	219	11.030	-2.293	26.081	1.00	37.10	T
	ATOM 7619	OH2	WAT	T	225	7.449	-9.230	35.544	1.00	45.80	T
5	ATOM 7620	OH2	WAT	T	226	10.479	-7.325	36.925	1.00	40.53	T
	ATOM 7632	OH2	WAT	T	263	16.989	-4.269	24.857	1.00	37.79	T
	ATOM 7633	OH2	WAT	T	264	16.818	-0.589	23.119	1.00	33.03	T
	ATOM 7634	OH2	WAT	T	265	12.877	-2.966	24.468	1.00	44.25	T
	ATOM 7637	OH2	WAT	T	268	15.829	-10.496	25.604	1.00	39.46	T
10	ATOM 7638	OH2	WAT	T	269	12.401	-18.158	31.715	1.00	28.89	T
	ATOM 7669	OH2	WAT	T	341	6.084	-13.571	24.399	1.00	44.58	T
	ATOM 7670	OH2	WAT	T	342	12.132	-14.509	26.051	1.00	36.17	T
	ATOM 7723	OH2	WAT	T	439	10.138	-4.873	30.054	1.00	32.06	T

15 Table 2

Three-dimensional coordinate of the complex of human hematopoietic PGDS with magnesium and glutathione

	ATOM 4966	N	TYR	A	8	24.798	32.294	34.444	1.00	27.67	A
20	ATOM 4967	CA	TYR	A	8	23.375	32.556	34.622	1.00	27.57	A
	ATOM 4968	CB	TYR	A	8	22.609	31.228	34.679	1.00	26.91	A
	ATOM 4969	CG	TYR	A	8	21.105	31.363	34.647	1.00	26.02	A
	ATOM 4970	CD1	TYR	A	8	20.462	31.990	33.580	1.00	25.80	A
	ATOM 4971	CE1	TYR	A	8	19.075	32.097	33.536	1.00	25.34	A
25	ATOM 4972	CD2	TYR	A	8	20.319	30.843	35.674	1.00	25.72	A

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	ATOM 4973	CE2	TYR	A	8	18.935	30.943	35.642	1.00	25.34	A
	ATOM 4974	CZ	TYR	A	8	18.315	31.571	34.570	1.00	25.28	A
	ATOM 4975	OH	TYR	A	8	16.945	31.672	34.539	1.00	24.76	A
	ATOM 4976	C	TYR	A	8	23.147	33.349	35.907	1.00	28.01	A
5	ATOM 4977	O	TYR	A	8	24.086	33.591	36.667	1.00	28.14	A
	ATOM 4978	N	PHE	A	9	21.906	33.767	36.140	1.00	28.37	A
	ATOM 4979	CA	PHE	A	9	21.572	34.518	37.349	1.00	28.74	A
	ATOM 4980	CB	PHE	A	9	20.161	35.097	37.247	1.00	28.79	A
	ATOM 4981	CG	PHE	A	9	20.034	36.202	36.236	1.00	29.08	A
10	ATOM 4982	CD1	PHE	A	9	19.031	36.169	35.273	1.00	29.16	A
	ATOM 4983	CD2	PHE	A	9	20.917	37.276	36.250	1.00	29.06	A
	ATOM 4984	CE1	PHE	A	9	18.905	37.192	34.335	1.00	29.23	A
	ATOM 4985	CE2	PHE	A	9	20.800	38.303	35.319	1.00	29.41	A
	ATOM 4986	CZ	PHE	A	9	19.792	38.260	34.357	1.00	29.36	A
15	ATOM 4987	C	PHE	A	9	21.656	33.583	38.547	1.00	28.97	A
	ATOM 4988	O	PHE	A	9	21.790	32.369	38.385	1.00	29.03	A
	ATOM 4989	N	ASN	A	10	21.590	34.145	39.749	1.00	29.09	A
	ATOM 4990	CA	ASN	A	10	21.650	33.326	40.952	1.00	29.24	A
	ATOM 4991	CB	ASN	A	10	22.167	34.143	42.140	1.00	29.62	A
20	ATOM 4992	CG	ASN	A	10	22.162	33.350	43.434	1.00	30.03	A
	ATOM 4993	OD1	ASN	A	10	22.370	32.134	43.432	1.00	30.13	A
	ATOM 4994	ND2	ASN	A	10	21.936	34.037	44.548	1.00	30.35	A
	ATOM 4995	C	ASN	A	10	20.276	32.753	41.266	1.00	29.04	A
	ATOM 4996	O	ASN	A	10	19.516	33.318	42.049	1.00	29.10	A
25	ATOM 4997	N	MET	A	11	19.962	31.627	40.631	1.00	28.94	A

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	ATOM 4998	CA	MET	A	11	18.685	30.942	40.824	1.00	28.66	A
	ATOM 4999	CB	MET	A	11	17.514	31.854	40.429	1.00	29.86	A
	ATOM 5000	CG	MET	A	11	17.483	32.272	38.969	1.00	31.35	A
	ATOM 5001	SD	MET	A	11	16.034	33.301	38.540	1.00	33.72	A
5	ATOM 5002	CE	MET	A	11	16.695	34.947	38.769	1.00	33.16	A
	ATOM 5003	C	MET	A	11	18.663	29.681	39.972	1.00	27.66	A
	ATOM 5004	O	MET	A	11	19.541	29.479	39.139	1.00	27.28	A
	ATOM 5005	N	ARG	A	12	17.674	28.822	40.193	1.00	26.89	A
	ATOM 5006	CA	ARG	A	12	17.568	27.598	39.410	1.00	25.99	A
10	ATOM 5007	CB	ARG	A	12	16.467	26.700	39.978	1.00	26.19	A
	ATOM 5008	CG	ARG	A	12	16.714	26.250	41.418	1.00	26.84	A
	ATOM 5009	CD	ARG	A	12	15.638	25.265	41.874	1.00	26.77	A
	ATOM 5010	NE	ARG	A	12	14.298	25.835	41.763	1.00	27.30	A
	ATOM 5011	CZ	ARG	A	12	13.794	26.737	42.598	1.00	27.44	A
15	ATOM 5012	NH1	ARG	A	12	14.518	27.177	43.621	1.00	27.56	A
	ATOM 5013	NH2	ARG	A	12	12.570	27.209	42.404	1.00	27.81	A
	ATOM 5014	C	ARG	A	12	17.236	28.011	37.977	1.00	25.35	A
	ATOM 5015	O	ARG	A	12	18.030	27.800	37.065	1.00	25.01	A
	ATOM 5016	N	GLY	A	13	16.062	28.607	37.797	1.00	24.64	A
20	ATOM 5017	CA	GLY	A	13	15.645	29.067	36.485	1.00	23.90	A
	ATOM 5018	C	GLY	A	13	15.900	28.126	35.326	1.00	23.52	A
	ATOM 5019	O	GLY	A	13	15.728	26.911	35.437	1.00	23.18	A
	ATOM 5020	N	ARG	A	14	16.333	28.696	34.205	1.00	22.72	A
	ATOM 5021	CA	ARG	A	14	16.592	27.920	32.998	1.00	22.38	A
25	ATOM 5022	CB	ARG	A	14	16.417	28.824	31.781	1.00	22.47	A

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	ATOM 5023	CG	ARG	A	14	15.004	29.342	31.659	1.00	22.96	A
	ATOM 5024	CD	ARG	A	14	14.807	30.214	30.443	1.00	23.81	A
	ATOM 5025	NE	ARG	A	14	13.386	30.325	30.135	1.00	24.80	A
	ATOM 5026	CZ	ARG	A	14	12.680	29.375	29.529	1.00	25.43	A
5	ATOM 5027	NH1	ARG	A	14	13.267	28.245	29.154	1.00	25.67	A
	ATOM 5028	NH2	ARG	A	14	11.381	29.547	29.319	1.00	26.33	A
	ATOM 5029	C	ARG	A	14	17.946	27.221	32.940	1.00	21.87	A
	ATOM 5030	O	ARG	A	14	18.206	26.450	32.021	1.00	21.54	A
	ATOM 5031	N	ALA	A	15	18.811	27.474	33.914	1.00	21.26	A
10	ATOM 5032	CA	ALA	A	15	20.109	26.826	33.910	1.00	20.98	A
	ATOM 5033	CB	ALA	A	15	21.180	27.785	34.416	1.00	21.37	A
	ATOM 5034	C	ALA	A	15	20.106	25.567	34.761	1.00	20.63	A
	ATOM 5035	O	ALA	A	15	21.055	24.785	34.724	1.00	20.56	A
	ATOM 5036	N	GLU	A	16	19.040	25.361	35.524	1.00	20.39	A
15	ATOM 5037	CA	GLU	A	16	18.985	24.198	36.401	1.00	20.26	A
	ATOM 5038	CB	GLU	A	16	17.739	24.260	37.284	1.00	20.92	A
	ATOM 5039	CG	GLU	A	16	17.825	23.399	38.537	1.00	21.66	A
	ATOM 5040	CD	GLU	A	16	19.007	23.757	39.425	1.00	22.12	A
	ATOM 5041	OE1	GLU	A	16	19.405	24.943	39.461	1.00	22.58	A
20	ATOM 5042	OE2	GLU	A	16	19.537	22.850	40.097	1.00	22.29	A
	ATOM 5043	C	GLU	A	16	19.030	22.871	35.656	1.00	19.57	A
	ATOM 5044	O	GLU	A	16	19.665	21.924	36.121	1.00	19.37	A
	ATOM 5045	N	ILE	A	17	18.371	22.791	34.502	1.00	19.00	A
	ATOM 5046	CA	ILE	A	17	18.374	21.539	33.749	1.00	18.27	A
25	ATOM 5047	CB	ILE	A	17	17.459	21.621	32.483	1.00	18.13	A

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	ATOM 5048	CG2	ILE	A	17	17.933	22.726	31.549	1.00	17.76	A
	ATOM 5049	CG1	ILE	A	17	17.431	20.262	31.771	1.00	17.74	A
	ATOM 5050	CD1	ILE	A	17	16.815	19.144	32.603	1.00	17.40	A
	ATOM 5051	C	ILE	A	17	19.795	21.141	33.354	1.00	18.40	A
5	ATOM 5052	O	ILE	A	17	20.135	19.956	33.327	1.00	18.19	A
	ATOM 5242	N	TRP	A	39	24.784	42.507	34.947	1.00	44.42	A
	ATOM 5243	CA	TRP	A	39	24.103	41.994	33.763	1.00	44.13	A
	ATOM 5244	CB	TRP	A	39	22.630	41.726	34.082	1.00	44.08	A
	ATOM 5245	CG	TRP	A	39	21.834	41.243	32.905	1.00	44.04	A
10	ATOM 5246	CD2	TRP	A	39	22.234	40.267	31.932	1.00	43.94	A
	ATOM 5247	CE2	TRP	A	39	21.162	40.122	31.023	1.00	43.97	A
	ATOM 5248	CE3	TRP	A	39	23.391	39.500	31.741	1.00	43.89	A
	ATOM 5249	CD1	TRP	A	39	20.576	41.637	32.555	1.00	44.04	A
	ATOM 5250	NE1	TRP	A	39	20.166	40.970	31.427	1.00	44.07	A
15	ATOM 5251	CZ2	TRP	A	39	21.212	39.242	29.936	1.00	43.96	A
	ATOM 5252	CZ3	TRP	A	39	23.442	38.623	30.657	1.00	43.92	A
	ATOM 5253	CH2	TRP	A	39	22.356	38.503	29.770	1.00	43.91	A
	ATOM 5254	C	TRP	A	39	24.202	42.927	32.553	1.00	44.00	A
	ATOM 5255	O	TRP	A	39	24.614	42.507	31.472	1.00	43.93	A
20	ATOM 5256	N	PRO	A	40	23.828	44.207	32.720	1.00	43.84	A
	ATOM 5257	CD	PRO	A	40	23.435	44.869	33.978	1.00	43.81	A
	ATOM 5258	CA	PRO	A	40	23.881	45.178	31.622	1.00	43.62	A
	ATOM 5259	CB	PRO	A	40	23.764	46.516	32.347	1.00	43.72	A
	ATOM 5260	CG	PRO	A	40	22.860	46.182	33.488	1.00	43.84	A
25	ATOM 5261	C	PRO	A	40	25.141	45.091	30.760	1.00	43.33	A

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	ATOM 5262	O	PRO	A	40	25.059	45.100	29.533	1.00	43.30	A
	ATOM 5263	N	GLU	A	41	26.301	45.003	31.402	1.00	42.98	A
	ATOM 5264	CA	GLU	A	41	27.569	44.921	30.681	1.00	42.61	A
	ATOM 5265	CB	GLU	A	41	28.741	45.127	31.647	1.00	43.08	A
5	ATOM 5266	CG	GLU	A	41	30.113	44.941	31.007	1.00	43.66	A
	ATOM 5267	CD	GLU	A	41	30.405	45.969	29.924	1.00	44.03	A
	ATOM 5268	OE1	GLU	A	41	31.411	45.800	29.198	1.00	44.15	A
	ATOM 5269	OE2	GLU	A	41	29.633	46.946	29.804	1.00	44.31	A
	ATOM 5270	C	GLU	A	41	27.742	43.593	29.953	1.00	42.03	A
10	ATOM 5271	O	GLU	A	41	28.054	43.560	28.761	1.00	42.06	A
	ATOM 5272	N	ILE	A	42	27.541	42.501	30.681	1.00	41.22	A
	ATOM 5273	CA	ILE	A	42	27.682	41.162	30.124	1.00	40.49	A
	ATOM 5274	CB	ILE	A	42	27.419	40.098	31.209	1.00	40.55	A
	ATOM 5275	CG2	ILE	A	42	27.600	38.703	30.631	1.00	40.56	A
15	ATOM 5276	CG1	ILE	A	42	28.376	40.319	32.382	1.00	40.56	A
	ATOM 5277	CD1	ILE	A	42	28.048	39.497	33.608	1.00	40.65	A
	ATOM 5278	C	ILE	A	42	26.722	40.933	28.959	1.00	39.90	A
	ATOM 5279	O	ILE	A	42	27.076	40.294	27.971	1.00	39.65	A
	ATOM 5280	N	LYS	A	43	25.511	41.468	29.083	1.00	39.26	A
20	ATOM 5281	CA	LYS	A	43	24.485	41.321	28.055	1.00	38.70	A
	ATOM 5282	CB	LYS	A	43	23.218	42.066	28.482	1.00	38.64	A
	ATOM 5283	CG	LYS	A	43	22.040	41.922	27.529	1.00	38.63	A
	ATOM 5284	CD	LYS	A	43	20.862	42.769	27.995	1.00	38.51	A
	ATOM 5285	CE	LYS	A	43	19.702	42.725	27.010	1.00	38.59	A
25	ATOM 5286	NZ	LYS	A	43	19.088	41.374	26.908	1.00	38.47	A

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	ATOM 5287	C	LYS A	43	24.941	41.821	26.682	1.00	38.32	A
	ATOM 5288	O	LYS A	43	24.657	41.195	25.656	1.00	38.07	A
	ATOM 5328	N	GLY A	49	22.169	38.393	23.696	1.00	27.72	A
	ATOM 5329	CA	GLY A	49	21.892	39.053	24.959	1.00	26.80	A
5	ATOM 5330	C	GLY A	49	20.981	38.310	25.914	1.00	26.17	A
	ATOM 5331	O	GLY A	49	20.163	38.922	26.607	1.00	25.97	A
	ATOM 5332	N	LYS A	50	21.123	36.991	25.961	1.00	25.32	A
	ATOM 5333	CA	LYS A	50	20.301	36.179	26.845	1.00	24.71	A
	ATOM 5334	CB	LYS A	50	19.164	35.522	26.052	1.00	25.17	A
10	ATOM 5335	CG	LYS A	50	18.256	36.493	25.314	1.00	26.18	A
	ATOM 5336	CD	LYS A	50	17.362	37.263	26.267	1.00	26.58	A
	ATOM 5337	CE	LYS A	50	16.619	38.387	25.552	1.00	27.00	A
	ATOM 5338	NZ	LYS A	50	15.862	37.901	24.367	1.00	27.09	A
	ATOM 5339	C	LYS A	50	21.114	35.095	27.527	1.00	24.20	A
15	ATOM 5340	O	LYS A	50	22.118	34.625	26.994	1.00	23.51	A
	ATOM 5341	N	ILE A	51	20.672	34.705	28.716	1.00	23.62	A
	ATOM 5342	CA	ILE A	51	21.329	33.642	29.462	1.00	23.69	A
	ATOM 5343	CB	ILE A	51	22.023	34.170	30.743	1.00	23.40	A
	ATOM 5344	CG2	ILE A	51	23.331	34.852	30.373	1.00	23.31	A
20	ATOM 5345	CG1	ILE A	51	21.086	35.106	31.510	1.00	23.39	A
	ATOM 5346	CD1	ILE A	51	21.696	35.661	32.779	1.00	23.78	A
	ATOM 5347	C	ILE A	51	20.270	32.609	29.822	1.00	23.77	A
	ATOM 5348	O	ILE A	51	19.074	32.888	29.754	1.00	23.72	A
	ATOM 5349	N	PRO A	52	20.697	31.411	30.239	1.00	24.02	A
25	ATOM 5350	CD	PRO A	52	19.778	30.321	30.607	1.00	24.22	A

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	ATOM 5351	CA	PRO	A	52	22.089	30.979	30.378	1.00	24.24	A
	ATOM 5352	CB	PRO	A	52	21.958	29.708	31.211	1.00	24.34	A
	ATOM 5353	CG	PRO	A	52	20.692	29.124	30.659	1.00	24.40	A
	ATOM 5354	C	PRO	A	52	22.843	30.711	29.082	1.00	24.32	A
5	ATOM 5355	O	PRO	A	52	22.258	30.608	27.999	1.00	24.21	A
	ATOM 5356	N	ILE	A	53	24.160	30.614	29.214	1.00	24.37	A
	ATOM 5357	CA	ILE	A	53	25.030	30.287	28.099	1.00	24.60	A
	ATOM 5358	CB	ILE	A	53	25.771	31.517	27.524	1.00	24.79	A
	ATOM 5359	CG2	ILE	A	53	24.772	32.471	26.876	1.00	24.74	A
10	ATOM 5360	CG1	ILE	A	53	26.583	32.210	28.623	1.00	24.92	A
	ATOM 5361	CD1	ILE	A	53	27.597	33.207	28.088	1.00	25.21	A
	ATOM 5362	C	ILE	A	53	26.051	29.318	28.659	1.00	24.74	A
	ATOM 5363	O	ILE	A	53	26.312	29.312	29.864	1.00	24.56	A
	ATOM 5423	N	HIS	A	62	24.282	28.843	23.471	1.00	20.06	A
15	ATOM 5424	CA	HIS	A	62	23.143	29.461	24.151	1.00	19.14	A
	ATOM 5425	CB	HIS	A	62	22.885	30.885	23.631	1.00	19.13	A
	ATOM 5426	CG	HIS	A	62	22.437	30.944	22.205	1.00	19.63	A
	ATOM 5427	CD2	HIS	A	62	21.300	31.421	21.646	1.00	19.62	A
	ATOM 5428	ND1	HIS	A	62	23.222	30.509	21.159	1.00	20.17	A
20	ATOM 5429	CE1	HIS	A	62	22.592	30.721	20.018	1.00	19.92	A
	ATOM 5430	NE2	HIS	A	62	21.423	31.275	20.285	1.00	20.10	A
	ATOM 5431	C	HIS	A	62	21.887	28.607	24.010	1.00	18.09	A
	ATOM 5432	O	HIS	A	62	21.914	27.591	23.321	1.00	17.56	A
	ATOM 5433	N	GLN	A	63	20.804	29.046	24.659	1.00	17.49	A
25	ATOM 5434	CA	GLN	A	63	19.512	28.342	24.693	1.00	16.80	A

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	ATOM 5435	CB	GLN	A	63	19.042	27.971	23.285	1.00	17.09	A
	ATOM 5436	CG	GLN	A	63	18.397	29.137	22.515	1.00	17.33	A
	ATOM 5437	CD	GLN	A	63	17.113	29.658	23.165	1.00	17.51	A
	ATOM 5438	OE1	GLN	A	63	16.514	28.993	24.013	1.00	17.71	A
5	ATOM 5439	NE2	GLN	A	63	16.676	30.846	22.750	1.00	18.20	A
	ATOM 5440	C	GLN	A	63	19.621	27.095	25.575	1.00	16.48	A
	ATOM 5441	O	GLN	A	63	20.248	26.098	25.202	1.00	15.97	A
	ATOM 5442	N	SER	A	64	18.983	27.166	26.740	1.00	16.15	A
	ATOM 5443	CA	SER	A	64	19.038	26.099	27.733	1.00	16.55	A
10	ATOM 5444	CB	SER	A	64	18.163	26.463	28.948	1.00	16.41	A
	ATOM 5445	OG	SER	A	64	16.780	26.507	28.637	1.00	17.25	A
	ATOM 5446	C	SER	A	64	18.705	24.688	27.258	1.00	16.42	A
	ATOM 5447	O	SER	A	64	19.395	23.736	27.625	1.00	16.29	A
	ATOM 5448	N	LEU	A	65	17.661	24.545	26.449	1.00	16.61	A
15	ATOM 5449	CA	LEU	A	65	17.266	23.221	25.979	1.00	16.62	A
	ATOM 5450	CB	LEU	A	65	15.803	23.242	25.518	1.00	17.28	A
	ATOM 5451	CG	LEU	A	65	14.804	23.694	26.599	1.00	17.94	A
	ATOM 5452	CD1	LEU	A	65	13.381	23.514	26.100	1.00	18.29	A
	ATOM 5453	CD2	LEU	A	65	15.023	22.904	27.884	1.00	18.01	A
20	ATOM 5454	C	LEU	A	65	18.183	22.699	24.874	1.00	16.53	A
	ATOM 5455	O	LEU	A	65	18.384	21.484	24.739	1.00	16.69	A
	ATOM 5662	N	ASP	A	93	9.437	20.470	25.569	1.00	14.02	A
	ATOM 5663	CA	ASP	A	93	8.852	21.675	24.974	1.00	15.28	A
	ATOM 5664	CB	ASP	A	93	8.823	21.563	23.440	1.00	16.56	A
25	ATOM 5665	CG	ASP	A	93	10.139	22.002	22.800	1.00	18.16	A

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	ATOM 5666	OD1	ASP	A	93	10.212	22.113	21.549	1.00	19.71	A
	ATOM 5667	OD2	ASP	A	93	11.116	22.243	23.549	1.00	19.34	A
	ATOM 5668	C	ASP	A	93	7.457	22.002	25.521	1.00	15.10	A
	ATOM 5669	O	ASP	A	93	7.103	23.178	25.671	1.00	15.47	A
5	ATOM 5670	N	THR	A	94	6.662	20.973	25.813	1.00	14.79	A
	ATOM 5671	CA	THR	A	94	5.327	21.184	26.365	1.00	14.62	A
	ATOM 5672	CB	THR	A	94	4.568	19.838	26.465	1.00	14.82	A
	ATOM 5673	OG1	THR	A	94	4.196	19.423	25.140	1.00	14.81	A
	ATOM 5674	CG2	THR	A	94	3.298	19.969	27.309	1.00	15.03	A
10	ATOM 5675	C	THR	A	94	5.475	21.860	27.736	1.00	15.22	A
	ATOM 5676	O	THR	A	94	4.758	22.805	28.051	1.00	14.83	A
	ATOM 5677	N	LEU	A	95	6.424	21.390	28.533	1.00	15.45	A
	ATOM 5678	CA	LEU	A	95	6.664	21.978	29.846	1.00	16.14	A
	ATOM 5679	CB	LEU	A	95	7.663	21.130	30.630	1.00	16.28	A
15	ATOM 5680	CG	LEU	A	95	7.107	19.798	31.120	1.00	16.61	A
	ATOM 5681	CD1	LEU	A	95	8.245	18.898	31.594	1.00	16.85	A
	ATOM 5682	CD2	LEU	A	95	6.103	20.052	32.240	1.00	17.08	A
	ATOM 5683	C	LEU	A	95	7.215	23.388	29.693	1.00	16.49	A
	ATOM 5684	O	LEU	A	95	6.745	24.327	30.344	1.00	16.45	A
20	ATOM 5685	N	ASP	A	96	8.208	23.540	28.823	1.00	16.67	A
	ATOM 5686	CA	ASP	A	96	8.824	24.850	28.621	1.00	17.83	A
	ATOM 5687	CB	ASP	A	96	10.001	24.736	27.646	1.00	18.40	A
	ATOM 5688	CG	ASP	A	96	11.004	25.860	27.815	1.00	19.35	A
	ATOM 5689	OD1	ASP	A	96	11.519	26.027	28.946	1.00	20.31	A
25	ATOM 5690	OD2	ASP	A	96	11.278	26.572	26.827	1.00	19.91	A

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	ATOM 5691	C	ASP	A	96	7.817	25.883	28.119	1.00	18.10	A
	ATOM 5692	O	ASP	A	96	7.850	27.046	28.536	1.00	17.78	A
	ATOM 5693	N	ASP	A	97	6.918	25.464	27.230	1.00	18.27	A
	ATOM 5694	CA	ASP	A	97	5.902	26.376	26.700	1.00	18.83	A
5	ATOM 5695	CB	ASP	A	97	4.957	25.644	25.741	1.00	19.25	A
	ATOM 5696	CG	ASP	A	97	5.582	25.365	24.386	1.00	20.04	A
	ATOM 5697	OD1	ASP	A	97	4.980	24.595	23.611	1.00	20.50	A
	ATOM 5698	OD2	ASP	A	97	6.660	25.914	24.085	1.00	20.61	A
	ATOM 5699	C	ASP	A	97	5.070	26.968	27.835	1.00	18.89	A
10	ATOM 5700	O	ASP	A	97	4.828	28.175	27.878	1.00	18.39	A
	ATOM 5701	N	PHE	A	98	4.630	26.107	28.750	1.00	19.13	A
	ATOM 5702	CA	PHE	A	98	3.814	26.547	29.875	1.00	19.65	A
	ATOM 5703	CB	PHE	A	98	3.311	25.342	30.686	1.00	20.03	A
	ATOM 5704	CG	PHE	A	98	2.426	25.718	31.854	1.00	20.47	A
15	ATOM 5705	CD1	PHE	A	98	1.249	26.436	31.650	1.00	20.90	A
	ATOM 5706	CD2	PHE	A	98	2.794	25.390	33.159	1.00	20.78	A
	ATOM 5707	CE1	PHE	A	98	0.451	26.827	32.732	1.00	21.07	A
	ATOM 5708	CE2	PHE	A	98	2.007	25.773	34.246	1.00	21.32	A
	ATOM 5709	CZ	PHE	A	98	0.837	26.495	34.035	1.00	21.00	A
20	ATOM 5710	C	PHE	A	98	4.598	27.495	30.776	1.00	20.02	A
	ATOM 5711	O	PHE	A	98	4.125	28.583	31.089	1.00	20.09	A
	ATOM 5712	N	MET	A	99	5.793	27.090	31.195	1.00	20.31	A
	ATOM 5713	CA	MET	A	99	6.607	27.937	32.064	1.00	21.46	A
	ATOM 5714	CB	MET	A	99	7.934	27.249	32.397	1.00	21.92	A
25	ATOM 5715	CG	MET	A	99	7.805	25.906	33.110	1.00	22.64	A

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	ATOM 5716	SD	MET	A	99	6.818	25.981	34.620	1.00	23.36	A
	ATOM 5717	CE	MET	A	99	7.919	26.938	35.719	1.00	23.75	A
	ATOM 5718	C	MET	A	99	6.885	29.294	31.416	1.00	21.88	A
	ATOM 5719	O	MET	A	99	6.921	30.321	32.101	1.00	21.92	A
5	ATOM 5720	N	SER	A	100	7.068	29.297	30.097	1.00	22.34	A
	ATOM 5721	CA	SER	A	100	7.356	30.530	29.359	1.00	23.09	A
	ATOM 5722	CB	SER	A	100	7.848	30.196	27.946	1.00	22.97	A
	ATOM 5723	OG	SER	A	100	9.105	29.535	27.992	1.00	22.88	A
	ATOM 5724	C	SER	A	100	6.169	31.486	29.280	1.00	23.87	A
10	ATOM 5725	O	SER	A	100	6.337	32.665	28.953	1.00	23.83	A
	ATOM 5726	N	CYS	A	101	4.973	30.980	29.569	1.00	24.59	A
	ATOM 5727	CA	CYS	A	101	3.769	31.812	29.551	1.00	25.73	A
	ATOM 5728	CB	CYS	A	101	2.504	30.950	29.642	1.00	26.18	A
	ATOM 5729	SG	CYS	A	101	2.072	30.045	28.134	1.00	27.14	A
15	ATOM 5730	C	CYS	A	101	3.764	32.802	30.711	1.00	26.07	A
	ATOM 5731	O	CYS	A	101	3.164	33.869	30.611	1.00	26.17	A
	ATOM 5732	N	PHE	A	102	4.424	32.452	31.814	1.00	26.61	A
	ATOM 5733	CA	PHE	A	102	4.448	33.344	32.969	1.00	27.42	A
	ATOM 5734	CB	PHE	A	102	4.968	32.621	34.218	1.00	27.19	A
20	ATOM 5735	CG	PHE	A	102	4.090	31.491	34.683	1.00	26.99	A
	ATOM 5736	CD1	PHE	A	102	4.118	30.261	34.035	1.00	26.96	A
	ATOM 5737	CD2	PHE	A	102	3.232	31.657	35.769	1.00	27.14	A
	ATOM 5738	CE1	PHE	A	102	3.308	29.205	34.459	1.00	27.01	A
	ATOM 5739	CE2	PHE	A	102	2.418	30.609	36.202	1.00	26.99	A
25	ATOM 5740	CZ	PHE	A	102	2.456	29.378	35.542	1.00	27.14	A

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	ATOM 5741	C	PHE A 102	5.298	34.587	32.719	1.00	27.95	A
	ATOM 5742	O	PHE A 102	6.423	34.495	32.237	1.00	27.67	A
	ATOM 5743	N	PRO A 103	4.761	35.774	33.045	1.00	28.91	A
	ATOM 5744	CD	PRO A 103	3.381	36.039	33.496	1.00	29.00	A
5	ATOM 5745	CA	PRO A 103	5.496	37.027	32.845	1.00	29.76	A
	ATOM 5746	CB	PRO A 103	4.381	38.061	32.792	1.00	29.51	A
	ATOM 5747	CG	PRO A 103	3.410	37.534	33.798	1.00	29.21	A
	ATOM 5748	C	PRO A 103	6.470	37.276	33.995	1.00	30.76	A
	ATOM 5749	O	PRO A 103	6.244	38.155	34.828	1.00	30.85	A
10	ATOM 5750	N	TRP A 104	7.555	36.508	34.027	1.00	31.83	A
	ATOM 5751	CA	TRP A 104	8.551	36.628	35.089	1.00	33.11	A
	ATOM 5752	CB	TRP A 104	9.647	35.572	34.917	1.00	32.91	A
	ATOM 5753	CG	TRP A 104	9.124	34.178	34.737	1.00	32.96	A
	ATOM 5754	CD2	TRP A 104	8.713	33.275	35.772	1.00	32.96	A
15	ATOM 5755	CE2	TRP A 104	8.269	32.092	35.141	1.00	33.00	A
	ATOM 5756	CE3	TRP A 104	8.677	33.351	37.174	1.00	33.00	A
	ATOM 5757	CD1	TRP A 104	8.918	33.525	33.555	1.00	32.88	A
	ATOM 5758	NE1	TRP A 104	8.405	32.271	33.789	1.00	32.93	A
	ATOM 5759	CZ2	TRP A 104	7.792	30.992	35.862	1.00	33.01	A
20	ATOM 5760	CZ3	TRP A 104	8.201	32.255	37.890	1.00	33.07	A
	ATOM 5761	CH2	TRP A 104	7.766	31.093	37.231	1.00	32.98	A
	ATOM 5762	C	TRP A 104	9.205	38.003	35.194	1.00	34.03	A
	ATOM 5763	O	TRP A 104	9.515	38.460	36.291	1.00	34.18	A
	ATOM 5764	N	ALA A 105	9.414	38.657	34.055	1.00	35.15	A
25	ATOM 5765	CA	ALA A 105	10.052	39.972	34.038	1.00	36.46	A

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	ATOM 5766	CB	ALA A 105	10.943	40.095	32.804	1.00	36.36	A
	ATOM 5767	C	ALA A 105	9.054	41.128	34.075	1.00	37.41	A
	ATOM 5768	O	ALA A 105	9.450	42.294	34.080	1.00	37.56	A
	ATOM 5769	N	GLU A 106	7.765	40.806	34.101	1.00	38.52	A
5	ATOM 5770	CA	GLU A 106	6.723	41.828	34.133	1.00	39.67	A
	ATOM 5771	CB	GLU A 106	5.344	41.166	34.069	1.00	39.95	A
	ATOM 5772	CG	GLU A 106	4.165	42.130	34.045	1.00	40.21	A
	ATOM 5773	CD	GLU A 106	4.304	43.209	32.989	1.00	40.48	A
	ATOM 5774	OE1	GLU A 106	4.932	44.251	33.276	1.00	40.68	A
10	ATOM 5775	OE2	GLU A 106	3.796	43.014	31.864	1.00	40.58	A
	ATOM 5776	C	GLU A 106	6.819	42.701	35.381	1.00	40.42	A
	ATOM 5777	O	GLU A 106	6.609	42.231	36.500	1.00	40.56	A
	ATOM 5778	N	LYS A 107	7.136	43.978	35.189	1.00	41.30	A
	ATOM 5779	CA	LYS A 107	7.250	44.895	36.315	1.00	42.22	A
15	ATOM 5780	CB	LYS A 107	8.092	46.110	35.927	1.00	42.33	A
	ATOM 5781	CG	LYS A 107	9.587	45.866	36.016	1.00	42.56	A
	ATOM 5782	CD	LYS A 107	10.000	45.596	37.457	1.00	42.79	A
	ATOM 5783	CE	LYS A 107	11.501	45.396	37.583	1.00	42.86	A
	ATOM 5784	NZ	LYS A 107	12.264	46.598	37.132	1.00	43.08	A
20	ATOM 5785	C	LYS A 107	5.890	45.343	36.831	1.00	42.73	A
	ATOM 5786	O	LYS A 107	5.719	45.571	38.030	1.00	42.99	A
	ATOM 5787	N	LYS A 108	4.925	45.465	35.927	1.00	43.26	A
	ATOM 5788	CA	LYS A 108	3.575	45.875	36.299	1.00	43.78	A
	ATOM 5789	CB	LYS A 108	2.734	46.106	35.041	1.00	43.97	A
25	ATOM 5790	CG	LYS A 108	3.322	47.146	34.099	1.00	44.32	A

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	ATOM 5791	CD	LYS A 108	2.459	47.357	32.862	1.00	44.57	A
	ATOM 5792	CE	LYS A 108	2.469	46.142	31.950	1.00	44.80	A
	ATOM 5793	NZ	LYS A 108	1.672	46.386	30.716	1.00	45.09	A
	ATOM 5794	C	LYS A 108	2.937	44.793	37.169	1.00	44.07	A
5	ATOM 5795	O	LYS A 108	2.342	43.841	36.662	1.00	44.03	A
	ATOM 5796	N	GLN A 109	3.069	44.954	38.483	1.00	44.42	A
	ATOM 5797	CA	GLN A 109	2.535	44.001	39.453	1.00	44.80	A
	ATOM 5798	CB	GLN A 109	2.686	44.569	40.870	1.00	45.10	A
	ATOM 5799	CG	GLN A 109	2.511	43.547	41.989	1.00	45.66	A
10	ATOM 5800	CD	GLN A 109	3.703	42.612	42.129	1.00	45.85	A
	ATOM 5801	OE1	GLN A 109	3.740	41.763	43.022	1.00	46.01	A
	ATOM 5802	NE2	GLN A 109	4.688	42.767	41.247	1.00	46.00	A
	ATOM 5803	C	GLN A 109	1.070	43.648	39.197	1.00	44.83	A
	ATOM 5804	O	GLN A 109	0.675	42.484	39.288	1.00	44.88	A
15	ATOM 5805	N	ASP A 110	0.267	44.656	38.876	1.00	44.78	A
	ATOM 5806	CA	ASP A 110	-1.153	44.451	38.616	1.00	44.83	A
	ATOM 5807	CB	ASP A 110	-1.816	45.784	38.257	1.00	45.28	A
	ATOM 5808	CG	ASP A 110	-1.243	46.399	36.992	1.00	45.63	A
	ATOM 5809	OD1	ASP A 110	-0.023	46.675	36.958	1.00	45.86	A
20	ATOM 5810	OD2	ASP A 110	-2.016	46.605	36.030	1.00	46.00	A
	ATOM 5811	C	ASP A 110	-1.399	43.437	37.496	1.00	44.67	A
	ATOM 5812	O	ASP A 110	-2.296	42.600	37.590	1.00	44.60	A
	ATOM 5813	N	VAL A 111	-0.597	43.519	36.439	1.00	44.34	A
	ATOM 5814	CA	VAL A 111	-0.730	42.621	35.298	1.00	44.07	A
25	ATOM 5815	CB	VAL A 111	-0.112	43.254	34.031	1.00	44.24	A

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	ATOM 5816	CG1	VAL	A	111	-0.338	42.352	32.828	1.00	44.21	A
	ATOM 5817	CG2	VAL	A	111	-0.718	44.628	33.794	1.00	44.30	A
	ATOM 5818	C	VAL	A	111	-0.058	41.273	35.556	1.00	43.75	A
	ATOM 5819	O	VAL	A	111	-0.571	40.229	35.157	1.00	43.61	A
5	ATOM 5820	N	LYS	A	112	1.088	41.305	36.227	1.00	43.49	A
	ATOM 5821	CA	LYS	A	112	1.834	40.093	36.534	1.00	43.29	A
	ATOM 5822	CB	LYS	A	112	3.161	40.452	37.207	1.00	43.21	A
	ATOM 5823	CG	LYS	A	112	4.040	39.255	37.531	1.00	43.24	A
	ATOM 5824	CD	LYS	A	112	5.354	39.686	38.160	1.00	43.22	A
10	ATOM 5825	CE	LYS	A	112	6.284	38.499	38.369	1.00	43.30	A
	ATOM 5826	NZ	LYS	A	112	7.585	38.911	38.962	1.00	43.09	A
	ATOM 5827	C	LYS	A	112	1.036	39.159	37.440	1.00	43.21	A
	ATOM 5828	O	LYS	A	112	0.865	37.976	37.136	1.00	43.01	A
	ATOM 5829	N	GLU	A	113	0.547	39.703	38.551	1.00	43.11	A
15	ATOM 5830	CA	GLU	A	113	-0.230	38.935	39.521	1.00	42.91	A
	ATOM 5831	CB	GLU	A	113	-0.676	39.849	40.670	1.00	43.22	A
	ATOM 5832	CG	GLU	A	113	-1.401	39.138	41.808	1.00	43.46	A
	ATOM 5833	CD	GLU	A	113	-0.473	38.290	42.660	1.00	43.66	A
	ATOM 5834	OE1	GLU	A	113	-0.951	37.683	43.644	1.00	43.73	A
20	ATOM 5835	OE2	GLU	A	113	0.738	38.232	42.348	1.00	43.75	A
	ATOM 5836	C	GLU	A	113	-1.460	38.288	38.884	1.00	42.68	A
	ATOM 5837	O	GLU	A	113	-1.799	37.142	39.187	1.00	42.56	A
	ATOM 5838	N	GLN	A	114	-2.121	39.031	38.002	1.00	42.28	A
	ATOM 5839	CA	GLN	A	114	-3.323	38.552	37.326	1.00	41.94	A
25	ATOM 5840	CB	GLN	A	114	-3.979	39.712	36.568	1.00	42.26	A

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	ATOM 5841	CG	GLN A 114	-5.404	39.462	36.083	1.00	42.72	A
	ATOM 5842	CD	GLN A 114	-5.470	38.624	34.821	1.00	42.97	A
	ATOM 5843	OE1	GLN A 114	-4.796	38.918	33.830	1.00	43.14	A
	ATOM 5844	NE2	GLN A 114	-6.302	37.584	34.841	1.00	43.11	A
5	ATOM 5845	C	GLN A 114	-3.030	37.396	36.372	1.00	41.52	A
	ATOM 5846	O	GLN A 114	-3.796	36.435	36.294	1.00	41.60	A
	ATOM 5847	N	MET A 115	-1.919	37.488	35.648	1.00	40.93	A
	ATOM 5848	CA	MET A 115	-1.549	36.439	34.706	1.00	40.35	A
	ATOM 5849	CB	MET A 115	-0.437	36.930	33.774	1.00	40.74	A
10	ATOM 5850	CG	MET A 115	-0.045	35.930	32.692	1.00	41.32	A
	ATOM 5851	SD	MET A 115	-1.436	35.356	31.684	1.00	42.13	A
	ATOM 5852	CE	MET A 115	-1.186	36.293	30.162	1.00	42.02	A
	ATOM 5853	C	MET A 115	-1.105	35.168	35.436	1.00	39.61	A
	ATOM 5854	O	MET A 115	-1.398	34.059	34.990	1.00	39.35	A
15	ATOM 5855	N	PHE A 116	-0.405	35.332	36.556	1.00	38.88	A
	ATOM 5856	CA	PHE A 116	0.056	34.188	37.335	1.00	38.26	A
	ATOM 5857	CB	PHE A 116	0.942	34.638	38.501	1.00	38.13	A
	ATOM 5858	CG	PHE A 116	2.406	34.690	38.170	1.00	37.93	A
	ATOM 5859	CD1	PHE A 116	2.893	35.593	37.232	1.00	37.95	A
20	ATOM 5860	CD2	PHE A 116	3.304	33.838	38.808	1.00	37.87	A
	ATOM 5861	CE1	PHE A 116	4.254	35.646	36.930	1.00	37.97	A
	ATOM 5862	CE2	PHE A 116	4.665	33.882	38.514	1.00	37.79	A
	ATOM 5863	CZ	PHE A 116	5.141	34.789	37.575	1.00	37.96	A
	ATOM 5864	C	PHE A 116	-1.114	33.385	37.886	1.00	38.04	A
25	ATOM 5865	O	PHE A 116	-1.147	32.161	37.769	1.00	37.81	A

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	ATOM 6152	N	TYR A 152	13.539	17.574	33.797	1.00	16.38	A
	ATOM 6153	CA	TYR A 152	12.825	18.812	33.538	1.00	16.80	A
	ATOM 6154	CB	TYR A 152	12.658	19.044	32.028	1.00	17.06	A
	ATOM 6155	CG	TYR A 152	12.623	20.514	31.669	1.00	17.96	A
5	ATOM 6156	CD1	TYR A 152	13.677	21.359	32.026	1.00	18.34	A
	ATOM 6157	CE1	TYR A 152	13.642	22.720	31.737	1.00	19.38	A
	ATOM 6158	CD2	TYR A 152	11.530	21.074	31.003	1.00	17.98	A
	ATOM 6159	CE2	TYR A 152	11.491	22.442	30.706	1.00	19.01	A
	ATOM 6160	CZ	TYR A 152	12.548	23.256	31.077	1.00	19.24	A
10	ATOM 6161	OH	TYR A 152	12.517	24.604	30.789	1.00	20.15	A
	ATOM 6162	C	TYR A 152	11.470	18.861	34.239	1.00	16.67	A
	ATOM 6163	O	TYR A 152	11.031	19.932	34.652	1.00	16.60	A
	ATOM 6164	N	TRP A 153	10.804	17.713	34.379	1.00	16.52	A
	ATOM 6165	CA	TRP A 153	9.518	17.691	35.071	1.00	16.67	A
15	ATOM 6166	CB	TRP A 153	8.870	16.299	35.002	1.00	16.89	A
	ATOM 6167	CG	TRP A 153	7.851	16.082	36.080	1.00	17.11	A
	ATOM 6168	CD2	TRP A 153	6.691	16.883	36.345	1.00	17.34	A
	ATOM 6169	CE2	TRP A 153	6.067	16.349	37.496	1.00	17.61	A
	ATOM 6170	CE3	TRP A 153	6.122	18.001	35.726	1.00	17.51	A
20	ATOM 6171	CD1	TRP A 153	7.879	15.120	37.053	1.00	17.56	A
	ATOM 6172	NE1	TRP A 153	6.815	15.278	37.906	1.00	17.47	A
	ATOM 6173	CZ2	TRP A 153	4.893	16.893	38.038	1.00	17.62	A
	ATOM 6174	CZ3	TRP A 153	4.954	18.548	36.264	1.00	17.52	A
	ATOM 6175	CH2	TRP A 153	4.352	17.990	37.410	1.00	17.93	A
25	ATOM 6176	C	TRP A 153	9.719	18.073	36.540	1.00	16.90	A

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	ATOM 6177	O	TRP A 153	8.963	18.874	37.101	1.00	16.93	A
	ATOM 6178	N	GLU A 154	10.746	17.502	37.156	1.00	16.92	A
	ATOM 6179	CA	GLU A 154	11.035	17.762	38.561	1.00	17.77	A
	ATOM 6180	CB	GLU A 154	12.168	16.846	39.037	1.00	18.50	A
5	ATOM 6181	CG	GLU A 154	12.341	16.793	40.555	1.00	20.34	A
	ATOM 6182	CD	GLU A 154	13.143	17.942	41.115	1.00	21.37	A
	ATOM 6183	OE1	GLU A 154	13.106	18.142	42.352	1.00	22.31	A
	ATOM 6184	OE2	GLU A 154	13.825	18.645	40.336	1.00	22.41	A
	ATOM 6185	C	GLU A 154	11.409	19.223	38.779	1.00	17.80	A
10	ATOM 6186	O	GLU A 154	10.992	19.841	39.765	1.00	17.40	A
	ATOM 6187	N	ILE A 155	12.189	19.766	37.848	1.00	17.91	A
	ATOM 6188	CA	ILE A 155	12.632	21.158	37.916	1.00	18.46	A
	ATOM 6189	CB	ILE A 155	13.704	21.442	36.837	1.00	18.42	A
	ATOM 6190	CG2	ILE A 155	13.999	22.953	36.754	1.00	18.94	A
15	ATOM 6191	CG1	ILE A 155	14.972	20.643	37.160	1.00	18.56	A
	ATOM 6192	CD1	ILE A 155	16.070	20.752	36.113	1.00	17.73	A
	ATOM 6193	C	ILE A 155	11.468	22.133	37.748	1.00	18.60	A
	ATOM 6194	O	ILE A 155	11.320	23.084	38.527	1.00	18.55	A
	ATOM 6195	N	CYS A 156	10.640	21.901	36.734	1.00	18.62	A
20	ATOM 6196	CA	CYS A 156	9.495	22.768	36.498	1.00	19.08	A
	ATOM 6197	CB	CYS A 156	8.808	22.418	35.170	1.00	19.21	A
	ATOM 6198	SG	CYS A 156	9.783	22.809	33.694	1.00	20.15	A
	ATOM 6199	C	CYS A 156	8.479	22.675	37.633	1.00	18.95	A
	ATOM 6200	O	CYS A 156	7.950	23.689	38.082	1.00	19.21	A
25	ATOM 6201	N	SER A 157	8.210	21.461	38.108	1.00	18.70	A

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	ATOM 6202	CA	SER A 157	7.229	21.301	39.175	1.00	18.57	A
	ATOM 6203	CB	SER A 157	6.890	19.820	39.388	1.00	18.17	A
	ATOM 6204	OG	SER A 157	8.042	19.055	39.674	1.00	18.09	A
	ATOM 6205	C	SER A 157	7.715	21.933	40.476	1.00	18.73	A
5	ATOM 6206	O	SER A 157	6.911	22.420	41.269	1.00	18.90	A
	ATOM 6207	N	THR A 158	9.025	21.928	40.694	1.00	18.86	A
	ATOM 6208	CA	THR A 158	9.586	22.536	41.898	1.00	19.39	A
	ATOM 6209	CB	THR A 158	11.124	22.436	41.915	1.00	19.38	A
	ATOM 6210	OG1	THR A 158	11.513	21.058	41.992	1.00	19.86	A
10	ATOM 6211	CG2	THR A 158	11.697	23.181	43.111	1.00	19.72	A
	ATOM 6212	C	THR A 158	9.180	24.011	41.953	1.00	19.58	A
	ATOM 6213	O	THR A 158	8.727	24.502	42.989	1.00	19.55	A
	ATOM 6214	N	THR A 159	9.336	24.714	40.836	1.00	19.71	A
	ATOM 6215	CA	THR A 159	8.977	26.129	40.791	1.00	20.16	A
15	ATOM 6216	CB	THR A 159	9.553	26.810	39.531	1.00	20.13	A
	ATOM 6217	OG1	THR A 159	10.981	26.811	39.617	1.00	20.61	A
	ATOM 6218	CG2	THR A 159	9.067	28.255	39.425	1.00	20.46	A
	ATOM 6219	C	THR A 159	7.468	26.347	40.855	1.00	20.37	A
	ATOM 6220	O	THR A 159	6.996	27.261	41.529	1.00	20.42	A
20	ATOM 6221	N	LEU A 160	6.701	25.509	40.163	1.00	20.18	A
	ATOM 6222	CA	LEU A 160	5.258	25.651	40.195	1.00	20.20	A
	ATOM 6223	CB	LEU A 160	4.607	24.665	39.229	1.00	20.20	A
	ATOM 6224	CG	LEU A 160	4.790	24.985	37.742	1.00	20.36	A
	ATOM 6225	CD1	LEU A 160	4.148	23.883	36.919	1.00	20.38	A
25	ATOM 6226	CD2	LEU A 160	4.171	26.340	37.411	1.00	20.08	A

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	ATOM 6227	C	LEU A 160	4.720	25.430	41.607	1.00	20.21	A
	ATOM 6228	O	LEU A 160	3.812	26.133	42.043	1.00	19.87	A
	ATOM 6229	N	LEU A 161	5.290	24.459	42.321	1.00	20.19	A
	ATOM 6230	CA	LEU A 161	4.853	24.148	43.686	1.00	20.28	A
5	ATOM 6231	CB	LEU A 161	5.580	22.902	44.207	1.00	20.48	A
	ATOM 6232	CG	LEU A 161	5.015	21.562	43.713	1.00	20.77	A
	ATOM 6233	CD1	LEU A 161	6.014	20.435	43.957	1.00	20.74	A
	ATOM 6234	CD2	LEU A 161	3.700	21.283	44.419	1.00	20.80	A
	ATOM 6235	C	LEU A 161	5.048	25.312	44.655	1.00	20.60	A
10	ATOM 6236	O	LEU A 161	4.329	25.426	45.651	1.00	20.50	A
	ATOM 6237	N	VAL A 162	6.021	26.170	44.364	1.00	20.44	A
	ATOM 6238	CA	VAL A 162	6.282	27.335	45.207	1.00	20.53	A
	ATOM 6239	CB	VAL A 162	7.546	28.101	44.744	1.00	20.23	A
	ATOM 6240	CG1	VAL A 162	7.622	29.466	45.434	1.00	20.06	A
15	ATOM 6241	CG2	VAL A 162	8.792	27.291	45.050	1.00	19.98	A
	ATOM 6242	C	VAL A 162	5.097	28.290	45.150	1.00	21.05	A
	ATOM 6243	O	VAL A 162	4.711	28.879	46.160	1.00	21.34	A
	ATOM 6244	N	PHE A 163	4.524	28.452	43.963	1.00	21.34	A
	ATOM 6245	CA	PHE A 163	3.395	29.356	43.785	1.00	21.75	A
20	ATOM 6246	CB	PHE A 163	3.517	30.080	42.448	1.00	21.81	A
	ATOM 6247	CG	PHE A 163	4.798	30.832	42.290	1.00	22.12	A
	ATOM 6248	CD1	PHE A 163	5.912	30.223	41.723	1.00	22.14	A
	ATOM 6249	CD2	PHE A 163	4.904	32.147	42.735	1.00	22.21	A
	ATOM 6250	CE1	PHE A 163	7.114	30.915	41.598	1.00	22.33	A
25	ATOM 6251	CE2	PHE A 163	6.103	32.845	42.615	1.00	22.06	A

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	ATOM 6252	CZ	PHE A 163	7.211	32.232	42.048	1.00	22.23	A
	ATOM 6253	C	PHE A 163	2.035	28.679	43.866	1.00	21.93	A
	ATOM 6254	O	PHE A 163	1.016	29.351	44.006	1.00	22.09	A
	ATOM 6528	N	THR A 197	16.938	29.580	46.456	1.00	42.04	A
5	ATOM 6529	CA	THR A 197	16.335	30.780	45.882	1.00	42.10	A
	ATOM 6530	CB	THR A 197	17.042	31.183	44.574	1.00	41.93	A
	ATOM 6531	OG1	THR A 197	17.071	30.063	43.680	1.00	41.66	A
	ATOM 6532	CG2	THR A 197	18.466	31.642	44.858	1.00	41.90	A
	ATOM 6533	C	THR A 197	14.852	30.565	45.588	1.00	42.37	A
10	ATOM 6534	O	THR A 197	14.363	29.436	45.631	1.00	42.08	A
	ATOM 6535	N	LYS A 198	14.140	31.649	45.288	1.00	42.36	A
	ATOM 6536	CA	LYS A 198	12.712	31.566	44.992	1.00	42.71	A
	ATOM 6537	CB	LYS A 198	12.052	32.947	45.102	1.00	42.62	A
	ATOM 6538	CG	LYS A 198	10.532	32.914	44.946	1.00	42.36	A
15	ATOM 6539	CD	LYS A 198	9.902	34.305	44.974	1.00	42.26	A
	ATOM 6540	CE	LYS A 198	10.279	35.121	43.746	1.00	42.29	A
	ATOM 6541	NZ	LYS A 198	9.661	36.480	43.744	1.00	42.09	A
	ATOM 6542	C	LYS A 198	12.451	30.995	43.599	1.00	42.44	A
	ATOM 6543	O	LYS A 198	11.440	30.331	43.376	1.00	43.10	A
20	ATOM 6544	N	LEU A 199	13.359	31.257	42.664	1.00	42.38	A
	ATOM 6545	CA	LEU A 199	13.208	30.762	41.302	1.00	41.31	A
	ATOM 6546	CB	LEU A 199	13.021	31.929	40.328	1.00	41.79	A
	ATOM 6547	CG	LEU A 199	11.826	32.851	40.580	1.00	41.74	A
	ATOM 6548	CD1	LEU A 199	11.825	33.976	39.562	1.00	41.87	A
25	ATOM 6549	CD2	LEU A 199	10.537	32.054	40.500	1.00	41.99	A

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	ATOM 6550	C	LEU A 199	14.415	29.940	40.880	1.00	41.18	A
	ATOM 6551	O	LEU A 199	15.357	29.815	41.690	1.00	40.87	A
	ATOM 6552	OXT	LEU A 199	14.404	29.431	39.740	1.00	40.62	A
	ATOM 6613	N1	GSH H 200	14.652	30.753	26.106	1.00	31.06	H
5	ATOM 6614	CA1	GSH H 200	16.043	30.929	26.532	1.00	30.39	H
	ATOM 6615	C1	GSH H 200	16.615	29.624	27.134	1.00	29.87	H
	ATOM 6616	O11	GSH H 200	15.850	28.693	27.401	1.00	29.01	H
	ATOM 6617	O12	GSH H 200	17.912	29.630	27.407	1.00	29.27	H
	ATOM 6618	CB1	GSH H 200	16.079	32.017	27.617	1.00	30.85	H
10	ATOM 6619	CG1	GSH H 200	16.018	33.443	27.054	1.00	30.90	H
	ATOM 6620	CD1	GSH H 200	15.735	34.381	28.252	1.00	30.62	H
	ATOM 6621	OE1	GSH H 200	14.695	35.035	28.263	1.00	30.67	H
	ATOM 6622	N2	GSH H 200	16.666	34.424	29.226	1.00	30.63	H
	ATOM 6623	CA2	GSH H 200	16.479	35.316	30.387	1.00	30.99	H
15	ATOM 6624	C2	GSH H 200	17.327	36.467	30.245	1.00	31.16	H
	ATOM 6625	O2	GSH H 200	18.505	36.372	29.874	1.00	30.98	H
	ATOM 6626	CB2	GSH H 200	16.883	34.616	31.709	1.00	30.96	H
	ATOM 6627	SG2	GSH H 200	15.567	33.583	32.426	1.00	31.20	H
	ATOM 6628	N3	GSH H 200	16.793	37.649	30.634	1.00	31.83	H
20	ATOM 6629	CA3	GSH H 200	17.595	38.892	30.738	1.00	32.45	H
	ATOM 6630	C3	GSH H 200	17.196	39.860	29.638	1.00	32.93	H
	ATOM 6631	O31	GSH H 200	17.851	40.926	29.570	1.00	33.18	H
	ATOM 6632	O32	GSH H 200	16.268	39.526	28.858	1.00	33.08	H
	ATOM 6634	MG+2	MG2 M 902	10.400	26.589	23.001	1.00	23.91	M
25	ATOM 6641	OH2	WAT S 7	11.530	25.061	23.828	1.00	37.06	S

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	ATOM 6642	OH2 WAT S	8	9.540	27.210	24.684	1.00	24.57	S
	ATOM 6643	OH2 WAT S	9	9.510	28.276	22.036	1.00	26.85	S
	ATOM 6644	OH2 WAT S	10	11.074	26.182	21.146	1.00	25.39	S
	ATOM 6645	OH2 WAT S	11	8.769	25.220	22.701	1.00	23.15	S
5	ATOM 6646	OH2 WAT S	12	12.343	27.736	23.214	1.00	21.75	S
	ATOM 6655	OH2 WAT S	21	16.153	24.647	33.762	1.00	15.93	S
	ATOM 6660	OH2 WAT S	26	22.016	34.735	24.315	1.00	19.54	S
	ATOM 6690	OH2 WAT S	56	19.895	31.455	26.292	1.00	20.15	S
	ATOM 6722	OH2 WAT S	88	15.099	33.768	23.429	1.00	20.21	S
10	ATOM 6746	OH2 WAT S	112	13.586	26.219	37.252	1.00	28.05	S
	ATOM 6749	OH2 WAT S	115	29.682	31.074	30.423	1.00	32.25	S
	ATOM 6757	OH2 WAT S	123	20.931	25.748	41.633	1.00	32.02	S
	ATOM 6758	OH2 WAT S	124	17.734	33.757	22.543	1.00	19.10	S
	ATOM 6770	OH2 WAT S	136	13.426	24.600	39.459	1.00	28.07	S
15	ATOM 6774	OH2 WAT S	140	16.050	26.391	24.708	1.00	22.82	S
	ATOM 6782	OH2 WAT S	148	14.395	37.589	28.342	1.00	35.97	S
	ATOM 6811	OH2 WAT S	177	19.958	32.909	23.887	1.00	18.07	S
	ATOM 6829	OH2 WAT S	195	14.106	35.347	25.480	1.00	25.75	S
	ATOM 6840	OH2 WAT S	206	14.044	35.490	20.956	1.00	20.11	S
20	ATOM 6928	OH2 WAT S	294	25.213	29.402	36.456	1.00	21.97	S
	ATOM 6929	OH2 WAT S	295	4.780	29.656	25.498	1.00	28.39	S
	ATOM 6940	OH2 WAT S	306	11.910	36.992	22.272	1.00	27.44	S
	ATOM 7008	OH2 WAT S	374	19.731	28.119	43.144	1.00	34.76	S
	ATOM 7079	OH2 WAT S	445	9.001	41.153	37.697	1.00	40.98	S
25	ATOM 7085	OH2 WAT S	451	14.312	39.335	22.120	1.00	52.27	S

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	ATOM 7095	OH2 WAT S 461	11.445	36.299	24.804	1.00	39.65	S
	ATOM 7123	OH2 WAT S 489	11.366	30.498	26.166	1.00	37.93	S
	ATOM 7129	OH2 WAT S 495	16.228	23.406	21.692	1.00	34.70	S
	ATOM 7138	OH2 WAT S 504	21.673	36.938	40.112	1.00	39.58	S
5	ATOM 7140	OH2 WAT S 506	8.186	35.879	39.587	1.00	35.09	S
	ATOM 7155	OH2 WAT S 521	17.208	36.485	21.785	1.00	33.85	S
	ATOM 7179	OH2 WAT S 545	7.692	39.218	31.544	1.00	38.01	S
	ATOM 7184	OH2 WAT S 550	16.301	40.121	43.773	1.00	42.74	S
	ATOM 7205	OH2 WAT S 571	16.471	40.729	21.826	1.00	44.98	S
10	ATOM 7219	OH2 WAT S 585	12.552	26.597	33.929	1.00	43.65	S
	ATOM 7229	OH2 WAT S 595	17.756	38.966	20.182	1.00	39.29	S
	ATOM 7231	OH2 WAT S 597	13.596	27.392	25.614	1.00	33.67	S
	ATOM 7235	OH2 WAT S 601	8.227	29.798	24.106	1.00	42.88	S
	ATOM 7250	OH2 WAT S 616	12.430	28.404	38.196	1.00	28.06	S
15	ATOM 7302	OH2 WAT S 668	8.268	32.489	24.271	1.00	34.58	S
	ATOM 7306	OH2 WAT S 672	13.738	43.695	22.850	1.00	40.33	S
	ATOM 7350	OH2 WAT S 716	16.122	38.680	37.510	1.00	37.39	S
	ATOM 7351	OH2 WAT S 717	12.657	31.864	34.383	1.00	37.30	S
	ATOM 7362	OH2 WAT S 728	24.227	34.662	22.649	1.00	33.80	S
20	ATOM 7363	OH2 WAT S 729	25.788	32.632	21.734	1.00	31.91	S
	ATOM 7398	OH2 WAT S 764	15.402	25.563	30.917	1.00	22.67	S
	ATOM 7399	OH2 WAT S 765	13.051	32.782	31.072	1.00	31.89	S
	ATOM 7400	OH2 WAT S 766	10.600	32.486	30.037	1.00	38.06	S
	ATOM 7453	OH2 WAT S 818	10.407	33.035	26.315	1.00	34.27	S
25	ATOM 7454	OH2 WAT S 819	4.103	39.433	24.839	1.00	35.58	S

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	ATOM 7455	OH2	WAT	S	820	8.800	40.482	25.686	1.00	38.38	S
	ATOM 7466	OH2	WAT	S	831	22.905	42.140	23.725	1.00	34.87	S
	ATOM 7523	OH2	WAT	S	890	11.498	40.681	41.811	1.00	34.74	S
	ATOM 7533	OH2	WAT	S	901	21.231	36.504	45.050	1.00	40.93	S
5	ATOM 7540	OH2	WAT	S	908	16.196	42.111	32.687	1.00	37.19	S
	ATOM 7588	OH2	WAT	S	1234	13.747	22.487	22.995	1.00	32.97	S

Table 3

Three-dimensional structural coordinate of the complex of
 10 human hematopoietic PGDS with calcium, glutathione and
 9,11-dideoxy -9 α ,11 α -methanoepoxyprostaglandine F_{2 α} (U46)

	ATOM 4966	N	TYR	A	8	-2.271	-4.196	32.836	1.00	14.93	A
	ATOM 4967	CA	TYR	A	8	-0.858	-4.474	33.097	1.00	15.12	A
15	ATOM 4968	CB	TYR	A	8	-0.097	-3.155	33.272	1.00	14.72	A
	ATOM 4969	CG	TYR	A	8	1.411	-3.302	33.334	1.00	14.32	A
	ATOM 4970	CD1	TYR	A	8	2.128	-3.846	32.262	1.00	13.92	A
	ATOM 4971	CE1	TYR	A	8	3.518	-3.985	32.321	1.00	13.52	A
	ATOM 4972	CD2	TYR	A	8	2.125	-2.898	34.469	1.00	14.03	A
20	ATOM 4973	CE2	TYR	A	8	3.508	-3.032	34.539	1.00	13.52	A
	ATOM 4974	CZ	TYR	A	8	4.199	-3.577	33.461	1.00	13.52	A
	ATOM 4975	OH	TYR	A	8	5.563	-3.718	33.529	1.00	13.03	A
	ATOM 4976	C	TYR	A	8	-0.758	-5.293	34.384	1.00	15.52	A
	ATOM 4977	O	TYR	A	8	-1.775	-5.603	35.002	1.00	15.35	A
25	ATOM 4978	N	PHE	A	9	0.460	-5.652	34.782	1.00	15.96	A

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	ATOM 4979	CA	PHE	A	9	0.654	-6.400	36.021	1.00	16.41	A
	ATOM 4980	CB	PHE	A	9	2.049	-7.029	36.071	1.00	16.62	A
	ATOM 4981	CG	PHE	A	9	2.240	-8.149	35.092	1.00	17.03	A
	ATOM 4982	CD1	PHE	A	9	3.165	-8.035	34.055	1.00	17.22	A
5	ATOM 4983	CD2	PHE	A	9	1.497	-9.322	35.209	1.00	17.29	A
	ATOM 4984	CE1	PHE	A	9	3.352	-9.072	33.143	1.00	17.28	A
	ATOM 4985	CE2	PHE	A	9	1.671	-10.371	34.304	1.00	17.39	A
	ATOM 4986	CZ	PHE	A	9	2.603	-10.245	33.267	1.00	17.64	A
	ATOM 4987	C	PHE	A	9	0.495	-5.427	37.187	1.00	16.51	A
10	ATOM 4988	O	PHE	A	9	0.380	-4.220	36.975	1.00	16.43	A
	ATOM 4989	N	ASN	A	10	0.485	-5.951	38.410	1.00	16.68	A
	ATOM 4990	CA	ASN	A	10	0.345	-5.114	39.595	1.00	17.13	A
	ATOM 4991	CB	ASN	A	10	-0.235	-5.911	40.765	1.00	17.62	A
	ATOM 4992	CG	ASN	A	10	-0.251	-5.111	42.053	1.00	18.18	A
15	ATOM 4993	OD1	ASN	A	10	-0.602	-3.927	42.060	1.00	18.91	A
	ATOM 4994	ND2	ASN	A	10	0.120	-5.751	43.151	1.00	18.74	A
	ATOM 4995	C	ASN	A	10	1.695	-4.539	39.996	1.00	17.08	A
	ATOM 4996	O	ASN	A	10	2.278	-4.934	41.002	1.00	17.04	A
	ATOM 4997	N	MET	A	11	2.189	-3.607	39.189	1.00	16.98	A
20	ATOM 4998	CA	MET	A	11	3.467	-2.962	39.448	1.00	16.70	A
	ATOM 4999	CB	MET	A	11	4.626	-3.927	39.141	1.00	17.68	A
	ATOM 5000	CG	MET	A	11	4.630	-4.530	37.748	1.00	18.92	A
	ATOM 5001	SD	MET	A	11	6.178	-5.456	37.353	1.00	20.84	A
	ATOM 5002	CE	MET	A	11	5.595	-7.137	37.373	1.00	19.96	A
25	ATOM 5003	C	MET	A	11	3.561	-1.708	38.587	1.00	15.92	A

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	ATOM 5004	O	MET A	11	2.740	-1.512	37.702	1.00	15.49	A
	ATOM 5005	N	ARG A	12	4.531	-0.842	38.872	1.00	15.17	A
	ATOM 5006	CA	ARG A	12	4.697	0.372	38.084	1.00	14.70	A
	ATOM 5007	CB	ARG A	12	5.759	1.285	38.704	1.00	14.69	A
5	ATOM 5008	CG	ARG A	12	5.418	1.777	40.110	1.00	15.00	A
	ATOM 5009	CD	ARG A	12	6.413	2.825	40.594	1.00	14.97	A
	ATOM 5010	NE	ARG A	12	7.785	2.323	40.634	1.00	15.22	A
	ATOM 5011	CZ	ARG A	12	8.265	1.490	41.556	1.00	15.45	A
	ATOM 5012	NH1	ARG A	12	7.485	1.052	42.536	1.00	15.40	A
10	ATOM 5013	NH2	ARG A	12	9.533	1.096	41.502	1.00	15.26	A
	ATOM 5014	C	ARG A	12	5.136	-0.069	36.695	1.00	14.31	A
	ATOM 5015	O	ARG A	12	4.432	0.147	35.710	1.00	13.90	A
	ATOM 5016	N	GLY A	13	6.301	-0.708	36.639	1.00	13.97	A
	ATOM 5017	CA	GLY A	13	6.837	-1.202	35.388	1.00	13.65	A
15	ATOM 5018	C	GLY A	13	6.705	-0.260	34.207	1.00	13.50	A
	ATOM 5019	O	GLY A	13	6.938	0.941	34.321	1.00	13.35	A
	ATOM 5020	N	ARG A	14	6.309	-0.816	33.070	1.00	13.31	A
	ATOM 5021	CA	ARG A	14	6.179	-0.047	31.848	1.00	13.30	A
	ATOM 5022	CB	ARG A	14	6.431	-0.959	30.650	1.00	14.32	A
20	ATOM 5023	CG	ARG A	14	7.877	-1.395	30.542	1.00	16.00	A
	ATOM 5024	CD	ARG A	14	8.117	-2.259	29.325	1.00	17.28	A
	ATOM 5025	NE	ARG A	14	9.532	-2.265	28.979	1.00	18.88	A
	ATOM 5026	CZ	ARG A	14	10.134	-1.329	28.246	1.00	19.26	A
	ATOM 5027	NH1	ARG A	14	9.444	-0.304	27.762	1.00	19.28	A
25	ATOM 5028	NH2	ARG A	14	11.442	-1.408	28.014	1.00	20.21	A

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	ATOM 5029	C	ARG A	14	4.859	0.689	31.669	1.00	12.77	A
	ATOM 5030	O	ARG A	14	4.696	1.435	30.710	1.00	12.75	A
	ATOM 5031	N	ALA A	15	3.920	0.496	32.590	1.00	12.21	A
	ATOM 5032	CA	ALA A	15	2.624	1.159	32.493	1.00	11.48	A
5	ATOM 5033	CB	ALA A	15	1.531	0.245	33.019	1.00	11.52	A
	ATOM 5034	C	ALA A	15	2.596	2.464	33.261	1.00	10.95	A
	ATOM 5035	O	ALA A	15	1.780	3.352	32.977	1.00	10.86	A
	ATOM 5036	N	GLU A	16	3.490	2.580	34.238	1.00	10.32	A
	ATOM 5037	CA	GLU A	16	3.546	3.771	35.087	1.00	9.76	A
10	ATOM 5038	CB	GLU A	16	4.748	3.677	36.036	1.00	9.29	A
	ATOM 5039	CG	GLU A	16	4.648	4.565	37.277	1.00	8.91	A
	ATOM 5040	CD	GLU A	16	3.485	4.192	38.189	1.00	8.41	A
	ATOM 5041	OE1	GLU A	16	2.858	3.134	37.983	1.00	8.43	A
	ATOM 5042	OE2	GLU A	16	3.199	4.960	39.125	1.00	8.51	A
15	ATOM 5043	C	GLU A	16	3.590	5.084	34.303	1.00	9.64	A
	ATOM 5044	O	GLU A	16	2.999	6.071	34.730	1.00	9.63	A
	ATOM 5045	N	ILE A	17	4.287	5.096	33.166	1.00	9.45	A
	ATOM 5046	CA	ILE A	17	4.377	6.312	32.368	1.00	9.29	A
	ATOM 5047	CB	ILE A	17	5.333	6.139	31.150	1.00	9.25	A
20	ATOM 5048	CG2	ILE A	17	4.867	5.015	30.251	1.00	9.64	A
	ATOM 5049	CG1	ILE A	17	5.413	7.442	30.358	1.00	9.55	A
	ATOM 5050	CD1	ILE A	17	5.988	8.596	31.168	1.00	9.78	A
	ATOM 5051	C	ILE A	17	2.984	6.717	31.892	1.00	9.19	A
	ATOM 5052	O	ILE A	17	2.648	7.897	31.845	1.00	8.98	A
25	ATOM 5242	N	TRP A	39	-2.591	-14.181	33.457	1.00	37.71	A

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	ATOM 5243	CA	TRP	A	39	-1.830	-13.655	32.329	1.00	37.46	A
	ATOM 5244	CB	TRP	A	39	-0.376	-13.394	32.737	1.00	37.38	A
	ATOM 5245	CG	TRP	A	39	0.495	-12.956	31.594	1.00	37.31	A
	ATOM 5246	CD2	TRP	A	39	0.174	-11.987	30.583	1.00	37.22	A
5	ATOM 5247	CE2	TRP	A	39	1.277	-11.918	29.704	1.00	37.19	A
	ATOM 5248	CE3	TRP	A	39	-0.940	-11.171	30.336	1.00	37.22	A
	ATOM 5249	CD1	TRP	A	39	1.745	-13.416	31.295	1.00	37.27	A
	ATOM 5250	NE1	TRP	A	39	2.220	-12.801	30.160	1.00	37.23	A
	ATOM 5251	CZ2	TRP	A	39	1.300	-11.068	28.594	1.00	37.19	A
10	ATOM 5252	CZ3	TRP	A	39	-0.916	-10.323	29.230	1.00	37.17	A
	ATOM 5253	CH2	TRP	A	39	0.198	-10.281	28.374	1.00	37.16	A
	ATOM 5254	C	TRP	A	39	-1.866	-14.602	31.124	1.00	37.40	A
	ATOM 5255	O	TRP	A	39	-2.138	-14.177	30.003	1.00	37.29	A
	ATOM 5256	N	PRO	A	40	-1.597	-15.901	31.342	1.00	37.35	A
15	ATOM 5257	CD	PRO	A	40	-1.235	-16.548	32.616	1.00	37.43	A
	ATOM 5258	CA	PRO	A	40	-1.605	-16.881	30.251	1.00	37.26	A
	ATOM 5259	CB	PRO	A	40	-1.489	-18.212	30.987	1.00	37.31	A
	ATOM 5260	CG	PRO	A	40	-0.618	-17.854	32.153	1.00	37.40	A
	ATOM 5261	C	PRO	A	40	-2.843	-16.817	29.363	1.00	37.11	A
20	ATOM 5262	O	PRO	A	40	-2.739	-16.888	28.139	1.00	37.23	A
	ATOM 5263	N	GLU	A	41	-4.011	-16.677	29.981	1.00	36.89	A
	ATOM 5264	CA	GLU	A	41	-5.265	-16.614	29.236	1.00	36.63	A
	ATOM 5265	CB	GLU	A	41	-6.457	-16.755	30.188	1.00	37.02	A
	ATOM 5266	CG	GLU	A	41	-7.757	-17.156	29.501	1.00	37.64	A
25	ATOM 5267	CD	GLU	A	41	-7.734	-18.601	29.023	1.00	38.10	A

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	ATOM 5268	OE1	GLU	A	41	-8.709	-19.033	28.364	1.00	38.32	A
	ATOM 5269	OE2	GLU	A	41	-6.741	-19.307	29.311	1.00	38.26	A
	ATOM 5270	C	GLU	A	41	-5.381	-15.297	28.474	1.00	36.10	A
	ATOM 5271	O	GLU	A	41	-5.703	-15.281	27.285	1.00	36.26	A
5	ATOM 5272	N	ILE	A	42	-5.120	-14.194	29.166	1.00	35.28	A
	ATOM 5273	CA	ILE	A	42	-5.204	-12.874	28.553	1.00	34.47	A
	ATOM 5274	CB	ILE	A	42	-4.980	-11.773	29.597	1.00	34.57	A
	ATOM 5275	CG2	ILE	A	42	-5.152	-10.406	28.953	1.00	34.48	A
	ATOM 5276	CG1	ILE	A	42	-5.968	-11.952	30.750	1.00	34.54	A
10	ATOM 5277	CD1	ILE	A	42	-5.687	-11.076	31.944	1.00	34.74	A
	ATOM 5278	C	ILE	A	42	-4.173	-12.715	27.441	1.00	33.83	A
	ATOM 5279	O	ILE	A	42	-4.466	-12.161	26.384	1.00	33.69	A
	ATOM 5280	N	LYS	A	43	-2.968	-13.213	27.691	1.00	33.07	A
	ATOM 5281	CA	LYS	A	43	-1.879	-13.133	26.729	1.00	32.30	A
15	ATOM 5282	CB	LYS	A	43	-0.664	-13.899	27.258	1.00	32.18	A
	ATOM 5283	CG	LYS	A	43	0.536	-13.883	26.324	1.00	32.18	A
	ATOM 5284	CD	LYS	A	43	1.622	-14.833	26.798	1.00	32.02	A
	ATOM 5285	CE	LYS	A	43	2.795	-14.865	25.831	1.00	31.99	A
	ATOM 5286	NZ	LYS	A	43	3.484	-13.542	25.723	1.00	31.70	A
20	ATOM 5287	C	LYS	A	43	-2.267	-13.674	25.354	1.00	31.74	A
	ATOM 5288	O	LYS	A	43	-2.038	-13.022	24.333	1.00	31.67	A
	ATOM 5328	N	GLY	A	49	0.717	-10.483	22.236	1.00	21.45	A
	ATOM 5329	CA	GLY	A	49	0.900	-11.142	23.516	1.00	20.85	A
	ATOM 5330	C	GLY	A	49	1.735	-10.433	24.567	1.00	20.53	A
25	ATOM 5331	O	GLY	A	49	2.506	-11.072	25.276	1.00	20.53	A

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	ATOM 5332	N	LYS	A	50	1.590	-9.120	24.688	1.00	20.06	A
	ATOM 5333	CA	LYS	A	50	2.354	-8.390	25.686	1.00	19.66	A
	ATOM 5334	CB	LYS	A	50	3.683	-7.916	25.085	1.00	19.97	A
	ATOM 5335	CG	LYS	A	50	4.636	-9.061	24.812	1.00	20.63	A
5	ATOM 5336	CD	LYS	A	50	5.846	-8.644	24.024	1.00	21.03	A
	ATOM 5337	CE	LYS	A	50	6.699	-9.864	23.706	1.00	21.10	A
	ATOM 5338	NZ	LYS	A	50	5.873	-10.927	23.044	1.00	21.21	A
	ATOM 5339	C	LYS	A	50	1.601	-7.206	26.271	1.00	19.21	A
	ATOM 5340	O	LYS	A	50	0.713	-6.633	25.636	1.00	18.74	A
10	ATOM 5341	N	ILE	A	51	1.963	-6.852	27.497	1.00	18.42	A
	ATOM 5342	CA	ILE	A	51	1.354	-5.720	28.162	1.00	18.05	A
	ATOM 5343	CB	ILE	A	51	0.574	-6.149	29.414	1.00	18.14	A
	ATOM 5344	CG2	ILE	A	51	-0.755	-6.739	29.010	1.00	17.97	A
	ATOM 5345	CG1	ILE	A	51	1.404	-7.128	30.246	1.00	18.34	A
15	ATOM 5346	CD1	ILE	A	51	0.681	-7.613	31.494	1.00	18.26	A
	ATOM 5347	C	ILE	A	51	2.424	-4.699	28.538	1.00	17.67	A
	ATOM 5348	O	ILE	A	51	3.618	-5.012	28.572	1.00	17.72	A
	ATOM 5349	N	PRO	A	52	2.002	-3.473	28.874	1.00	17.15	A
	ATOM 5350	CD	PRO	A	52	2.906	-2.369	29.239	1.00	17.33	A
20	ATOM 5351	CA	PRO	A	52	0.610	-3.021	28.909	1.00	16.82	A
	ATOM 5352	CB	PRO	A	52	0.703	-1.736	29.713	1.00	16.81	A
	ATOM 5353	CG	PRO	A	52	1.968	-1.159	29.205	1.00	16.96	A
	ATOM 5354	C	PRO	A	52	-0.093	-2.777	27.584	1.00	16.60	A
	ATOM 5355	O	PRO	A	52	0.526	-2.674	26.526	1.00	16.29	A
25	ATOM 5356	N	ILE	A	53	-1.411	-2.678	27.672	1.00	16.36	A

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	ATOM 5357	CA	ILE A	53	-2.233	-2.361	26.522	1.00	16.17	A
	ATOM 5358	CB	ILE A	53	-2.992	-3.587	25.980	1.00	16.14	A
	ATOM 5359	CG2	ILE A	53	-2.000	-4.620	25.440	1.00	16.39	A
	ATOM 5360	CG1	ILE A	53	-3.875	-4.184	27.071	1.00	16.34	A
5	ATOM 5361	CD1	ILE A	53	-4.859	-5.218	26.544	1.00	16.22	A
	ATOM 5362	C	ILE A	53	-3.235	-1.325	27.015	1.00	15.98	A
	ATOM 5363	O	ILE A	53	-3.563	-1.277	28.202	1.00	15.70	A
	ATOM 5423	N	HIS A	62	-1.249	-1.093	22.011	1.00	11.78	A
	ATOM 5424	CA	HIS A	62	-0.158	-1.730	22.757	1.00	11.13	A
10	ATOM 5425	CB	HIS A	62	0.120	-3.150	22.240	1.00	11.01	A
	ATOM 5426	CG	HIS A	62	0.673	-3.202	20.848	1.00	10.84	A
	ATOM 5427	CD2	HIS A	62	1.903	-3.533	20.392	1.00	10.56	A
	ATOM 5428	ND1	HIS A	62	-0.087	-2.926	19.732	1.00	10.84	A
	ATOM 5429	CE1	HIS A	62	0.650	-3.090	18.648	1.00	10.55	A
15	ATOM 5430	NE2	HIS A	62	1.861	-3.458	19.021	1.00	10.75	A
	ATOM 5431	C	HIS A	62	1.112	-0.882	22.665	1.00	10.62	A
	ATOM 5432	O	HIS A	62	1.118	0.155	21.996	1.00	10.80	A
	ATOM 5433	N	GLN A	63	2.176	-1.337	23.332	1.00	10.07	A
	ATOM 5434	CA	GLN A	63	3.465	-0.641	23.377	1.00	9.39	A
20	ATOM 5435	CB	GLN A	63	3.957	-0.289	21.969	1.00	9.20	A
	ATOM 5436	CG	GLN A	63	4.702	-1.417	21.248	1.00	8.99	A
	ATOM 5437	CD	GLN A	63	5.911	-1.932	22.027	1.00	8.95	A
	ATOM 5438	OE1	GLN A	63	6.481	-1.220	22.858	1.00	8.52	A
	ATOM 5439	NE2	GLN A	63	6.315	-3.165	21.745	1.00	8.76	A
25	ATOM 5440	C	GLN A	63	3.324	0.618	24.223	1.00	8.90	A

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	ATOM 5441	O	GLN A	63	2.781	1.629	23.769	1.00	9.08	A
	ATOM 5442	N	SER A	64	3.830	0.554	25.452	1.00	8.48	A
	ATOM 5443	CA	SER A	64	3.708	1.668	26.396	1.00	8.06	A
	ATOM 5444	CB	SER A	64	4.440	1.342	27.706	1.00	7.67	A
5	ATOM 5445	OG	SER A	64	5.839	1.246	27.528	1.00	8.18	A
	ATOM 5446	C	SER A	64	4.143	3.045	25.902	1.00	7.75	A
	ATOM 5447	O	SER A	64	3.447	4.032	26.141	1.00	7.74	A
	ATOM 5448	N	LEU A	65	5.284	3.126	25.225	1.00	7.75	A
	ATOM 5449	CA	LEU A	65	5.754	4.424	24.752	1.00	7.47	A
10	ATOM 5450	CB	LEU A	65	7.224	4.346	24.359	1.00	7.66	A
	ATOM 5451	CG	LEU A	65	8.162	3.849	25.461	1.00	7.74	A
	ATOM 5452	CD1	LEU A	65	9.591	4.192	25.062	1.00	7.25	A
	ATOM 5453	CD2	LEU A	65	7.820	4.516	26.812	1.00	7.33	A
	ATOM 5454	C	LEU A	65	4.928	4.945	23.586	1.00	7.33	A
15	ATOM 5455	O	LEU A	65	4.768	6.151	23.426	1.00	7.33	A
	ATOM 5662	N	ASP A	93	13.523	7.274	24.597	1.00	7.43	A
	ATOM 5663	CA	ASP A	93	14.133	6.074	24.039	1.00	7.59	A
	ATOM 5664	CB	ASP A	93	14.267	6.190	22.520	1.00	7.58	A
	ATOM 5665	CG	ASP A	93	12.964	5.867	21.793	1.00	7.82	A
20	ATOM 5666	OD1	ASP A	93	12.977	5.837	20.550	1.00	8.49	A
	ATOM 5667	OD2	ASP A	93	11.937	5.640	22.466	1.00	7.73	A
	ATOM 5668	C	ASP A	93	15.494	5.763	24.674	1.00	7.65	A
	ATOM 5669	O	ASP A	93	15.839	4.597	24.858	1.00	8.00	A
	ATOM 5670	N	THR A	94	16.259	6.800	25.009	1.00	7.91	A
25	ATOM 5671	CA	THR A	94	17.561	6.608	25.646	1.00	8.08	A

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	ATOM 5672	CB	THR	A	94	18.281	7.963	25.879	1.00	8.13	A
	ATOM 5673	OG1	THR	A	94	18.619	8.547	24.617	1.00	8.31	A
	ATOM 5674	CG2	THR	A	94	19.557	7.772	26.701	1.00	8.08	A
	ATOM 5675	C	THR	A	94	17.361	5.905	26.993	1.00	8.54	A
5	ATOM 5676	O	THR	A	94	18.046	4.925	27.308	1.00	8.42	A
	ATOM 5677	N	LEU	A	95	16.424	6.410	27.788	1.00	8.76	A
	ATOM 5678	CA	LEU	A	95	16.137	5.804	29.079	1.00	9.53	A
	ATOM 5679	CB	LEU	A	95	15.107	6.642	29.851	1.00	9.33	A
	ATOM 5680	CG	LEU	A	95	15.647	7.972	30.383	1.00	9.50	A
10	ATOM 5681	CD1	LEU	A	95	14.517	8.827	30.949	1.00	9.22	A
	ATOM 5682	CD2	LEU	A	95	16.694	7.684	31.453	1.00	9.41	A
	ATOM 5683	C	LEU	A	95	15.618	4.377	28.879	1.00	9.79	A
	ATOM 5684	O	LEU	A	95	16.055	3.460	29.566	1.00	9.96	A
	ATOM 5685	N	ASP	A	96	14.709	4.200	27.920	1.00	10.44	A
15	ATOM 5686	CA	ASP	A	96	14.123	2.896	27.626	1.00	11.05	A
	ATOM 5687	CB	ASP	A	96	13.062	3.027	26.529	1.00	11.36	A
	ATOM 5688	CG	ASP	A	96	12.107	1.841	26.499	1.00	11.78	A
	ATOM 5689	OD1	ASP	A	96	11.640	1.431	27.579	1.00	12.41	A
	ATOM 5690	OD2	ASP	A	96	11.806	1.334	25.409	1.00	12.03	A
20	ATOM 5691	C	ASP	A	96	15.182	1.876	27.201	1.00	11.34	A
	ATOM 5692	O	ASP	A	96	15.169	0.734	27.650	1.00	11.33	A
	ATOM 5693	N	ASP	A	97	16.092	2.294	26.329	1.00	11.73	A
	ATOM 5694	CA	ASP	A	97	17.154	1.412	25.875	1.00	12.14	A
	ATOM 5695	CB	ASP	A	97	18.136	2.154	24.963	1.00	11.82	A
25	ATOM 5696	CG	ASP	A	97	17.599	2.373	23.544	1.00	11.92	A

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	ATOM 5697	OD1	ASP	A	97	18.280	3.083	22.784	1.00	11.78	A
	ATOM 5698	OD2	ASP	A	97	16.524	1.840	23.187	1.00	11.79	A
	ATOM 5699	C	ASP	A	97	17.924	0.865	27.084	1.00	12.59	A
	ATOM 5700	O	ASP	A	97	18.228	-0.326	27.150	1.00	12.62	A
5	ATOM 5701	N	PHE	A	98	18.242	1.731	28.041	1.00	13.02	A
	ATOM 5702	CA	PHE	A	98	18.992	1.296	29.219	1.00	13.80	A
	ATOM 5703	CB	PHE	A	98	19.449	2.500	30.047	1.00	13.80	A
	ATOM 5704	CG	PHE	A	98	20.332	2.127	31.203	1.00	14.07	A
	ATOM 5705	CD1	PHE	A	98	21.550	1.488	30.990	1.00	14.20	A
10	ATOM 5706	CD2	PHE	A	98	19.937	2.391	32.507	1.00	14.15	A
	ATOM 5707	CE1	PHE	A	98	22.358	1.115	32.064	1.00	14.32	A
	ATOM 5708	CE2	PHE	A	98	20.736	2.022	33.583	1.00	14.28	A
	ATOM 5709	CZ	PHE	A	98	21.948	1.384	33.361	1.00	14.12	A
	ATOM 5710	C	PHE	A	98	18.209	0.335	30.112	1.00	14.33	A
15	ATOM 5711	O	PHE	A	98	18.705	-0.739	30.467	1.00	14.62	A
	ATOM 5712	N	MET	A	99	16.992	0.722	30.482	1.00	14.73	A
	ATOM 5713	CA	MET	A	99	16.158	-0.120	31.329	1.00	15.34	A
	ATOM 5714	CB	MET	A	99	14.798	0.546	31.574	1.00	15.08	A
	ATOM 5715	CG	MET	A	99	14.878	1.932	32.202	1.00	14.94	A
20	ATOM 5716	SD	MET	A	99	15.699	1.910	33.803	1.00	14.67	A
	ATOM 5717	CE	MET	A	99	14.395	1.275	34.807	1.00	14.69	A
	ATOM 5718	C	MET	A	99	15.938	-1.489	30.691	1.00	16.11	A
	ATOM 5719	O	MET	A	99	15.882	-2.504	31.387	1.00	15.98	A
	ATOM 5720	N	SER	A	100	15.811	-1.516	29.366	1.00	16.74	A
25	ATOM 5721	CA	SER	A	100	15.576	-2.767	28.656	1.00	17.44	A

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	ATOM 5722	CB	SER A 100	15.116	-2.479	27.225	1.00	17.47	A
	ATOM 5723	OG	SER A 100	13.823	-1.884	27.234	1.00	17.51	A
	ATOM 5724	C	SER A 100	16.797	-3.681	28.656	1.00	18.04	A
	ATOM 5725	O	SER A 100	16.674	-4.888	28.436	1.00	18.07	A
5	ATOM 5726	N	CYS A 101	17.972	-3.111	28.912	1.00	18.65	A
	ATOM 5727	CA	CYS A 101	19.196	-3.905	28.964	1.00	19.36	A
	ATOM 5728	CB	CYS A 101	20.428	-3.006	29.108	1.00	19.22	A
	ATOM 5729	SG	CYS A 101	20.898	-2.082	27.630	1.00	20.13	A
	ATOM 5730	C	CYS A 101	19.167	-4.889	30.134	1.00	19.75	A
10	ATOM 5731	O	CYS A 101	19.772	-5.950	30.059	1.00	19.91	A
	ATOM 5732	N	PHE A 102	18.482	-4.533	31.218	1.00	20.31	A
	ATOM 5733	CA	PHE A 102	18.410	-5.420	32.376	1.00	21.09	A
	ATOM 5734	CB	PHE A 102	17.826	-4.693	33.594	1.00	20.83	A
	ATOM 5735	CG	PHE A 102	18.672	-3.551	34.087	1.00	20.72	A
15	ATOM 5736	CD1	PHE A 102	18.775	-2.376	33.344	1.00	20.56	A
	ATOM 5737	CD2	PHE A 102	19.374	-3.652	35.290	1.00	20.64	A
	ATOM 5738	CE1	PHE A 102	19.565	-1.313	33.788	1.00	20.64	A
	ATOM 5739	CE2	PHE A 102	20.170	-2.597	35.750	1.00	20.52	A
	ATOM 5740	CZ	PHE A 102	20.267	-1.423	34.996	1.00	20.66	A
20	ATOM 5741	C	PHE A 102	17.554	-6.645	32.060	1.00	21.79	A
	ATOM 5742	O	PHE A 102	16.490	-6.525	31.456	1.00	21.62	A
	ATOM 5743	N	PRO A 103	18.024	-7.844	32.450	1.00	22.58	A
	ATOM 5744	CD	PRO A 103	19.392	-8.117	32.928	1.00	22.84	A
	ATOM 5745	CA	PRO A 103	17.297	-9.098	32.211	1.00	23.41	A
25	ATOM 5746	CB	PRO A 103	18.415	-10.133	32.185	1.00	23.19	A

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	ATOM 5747	CG	PRO A 103	19.353	-9.611	33.222	1.00	23.10	A
	ATOM 5748	C	PRO A 103	16.272	-9.366	33.321	1.00	24.25	A
	ATOM 5749	O	PRO A 103	16.459	-10.248	34.160	1.00	24.19	A
	ATOM 5750	N	TRP A 104	15.191	-8.594	33.313	1.00	25.16	A
5	ATOM 5751	CA	TRP A 104	14.142	-8.722	34.313	1.00	26.25	A
	ATOM 5752	CB	TRP A 104	13.049	-7.673	34.072	1.00	25.95	A
	ATOM 5753	CG	TRP A 104	13.551	-6.261	33.946	1.00	25.64	A
	ATOM 5754	CD2	TRP A 104	13.907	-5.375	35.016	1.00	25.47	A
	ATOM 5755	CE2	TRP A 104	14.332	-4.162	34.429	1.00	25.40	A
10	ATOM 5756	CE3	TRP A 104	13.909	-5.488	36.412	1.00	25.27	A
	ATOM 5757	CD1	TRP A 104	13.770	-5.568	32.788	1.00	25.58	A
	ATOM 5758	NE1	TRP A 104	14.237	-4.307	33.070	1.00	25.45	A
	ATOM 5759	CZ2	TRP A 104	14.757	-3.067	35.193	1.00	25.38	A
	ATOM 5760	CZ3	TRP A 104	14.331	-4.398	37.173	1.00	25.16	A
15	ATOM 5761	CH2	TRP A 104	14.749	-3.205	36.560	1.00	25.21	A
	ATOM 5762	C	TRP A 104	13.511	-10.115	34.334	1.00	27.21	A
	ATOM 5763	O	TRP A 104	13.078	-10.597	35.383	1.00	27.22	A
	ATOM 5764	N	ALA A 105	13.472	-10.763	33.175	1.00	28.32	A
	ATOM 5765	CA	ALA A 105	12.872	-12.087	33.058	1.00	29.49	A
20	ATOM 5766	CB	ALA A 105	12.207	-12.226	31.697	1.00	29.48	A
	ATOM 5767	C	ALA A 105	13.853	-13.233	33.270	1.00	30.44	A
	ATOM 5768	O	ALA A 105	13.445	-14.391	33.354	1.00	30.58	A
	ATOM 5769	N	GLU A 106	15.140	-12.917	33.369	1.00	31.43	A
	ATOM 5770	CA	GLU A 106	16.147	-13.954	33.552	1.00	32.55	A
25	ATOM 5771	CB	GLU A 106	17.545	-13.338	33.620	1.00	32.51	A

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	ATOM 5772	CG	GLU A 106	18.634	-14.386	33.634	1.00	32.51	A
	ATOM 5773	CD	GLU A 106	18.498	-15.352	32.472	1.00	32.54	A
	ATOM 5774	OE1	GLU A 106	18.761	-16.555	32.662	1.00	32.34	A
	ATOM 5775	OE2	GLU A 106	18.129	-14.905	31.365	1.00	32.59	A
5	ATOM 5776	C	GLU A 106	15.913	-14.809	34.791	1.00	33.37	A
	ATOM 5777	O	GLU A 106	15.830	-14.294	35.908	1.00	33.46	A
	ATOM 5778	N	LYS A 107	15.813	-16.121	34.588	1.00	34.40	A
	ATOM 5779	CA	LYS A 107	15.592	-17.048	35.695	1.00	35.40	A
	ATOM 5780	CB	LYS A 107	14.830	-18.287	35.212	1.00	35.45	A
10	ATOM 5781	CG	LYS A 107	13.486	-17.992	34.553	1.00	35.72	A
	ATOM 5782	CD	LYS A 107	12.523	-17.293	35.497	1.00	35.84	A
	ATOM 5783	CE	LYS A 107	12.103	-18.197	36.639	1.00	36.12	A
	ATOM 5784	NZ	LYS A 107	11.273	-17.459	37.636	1.00	36.20	A
	ATOM 5785	C	LYS A 107	16.915	-17.471	36.336	1.00	36.00	A
15	ATOM 5786	O	LYS A 107	16.947	-17.902	37.490	1.00	36.10	A
	ATOM 5787	N	LYS A 108	18.003	-17.346	35.584	1.00	36.66	A
	ATOM 5788	CA	LYS A 108	19.325	-17.698	36.088	1.00	37.40	A
	ATOM 5789	CB	LYS A 108	20.295	-17.894	34.923	1.00	37.54	A
	ATOM 5790	CG	LYS A 108	19.855	-18.959	33.941	1.00	37.73	A
20	ATOM 5791	CD	LYS A 108	20.783	-19.026	32.748	1.00	37.95	A
	ATOM 5792	CE	LYS A 108	20.335	-20.101	31.781	1.00	38.07	A
	ATOM 5793	NZ	LYS A 108	21.226	-20.180	30.593	1.00	38.35	A
	ATOM 5794	C	LYS A 108	19.824	-16.576	36.992	1.00	37.85	A
	ATOM 5795	O	LYS A 108	20.361	-15.575	36.514	1.00	37.87	A
25	ATOM 5796	N	GLN A 109	19.650	-16.751	38.298	1.00	38.38	A

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	ATOM 5797	CA	GLN A 109	20.057	-15.742	39.274	1.00	38.89	A
	ATOM 5798	CB	GLN A 109	19.893	-16.287	40.696	1.00	39.27	A
	ATOM 5799	CG	GLN A 109	19.103	-15.372	41.621	1.00	39.77	A
	ATOM 5800	CD	GLN A 109	17.631	-15.280	41.236	1.00	40.04	A
5	ATOM 5801	OE1	GLN A 109	16.878	-14.472	41.791	1.00	40.13	A
	ATOM 5802	NE2	GLN A 109	17.214	-16.116	40.287	1.00	40.11	A
	ATOM 5803	C	GLN A 109	21.491	-15.264	39.081	1.00	38.96	A
	ATOM 5804	O	GLN A 109	21.755	-14.061	39.052	1.00	39.02	A
	ATOM 5805	N	ASP A 110	22.413	-16.211	38.951	1.00	39.02	A
10	ATOM 5806	CA	ASP A 110	23.826	-15.890	38.773	1.00	39.02	A
	ATOM 5807	CB	ASP A 110	24.631	-17.178	38.608	1.00	39.32	A
	ATOM 5808	CG	ASP A 110	24.226	-17.956	37.375	1.00	39.50	A
	ATOM 5809	OD1	ASP A 110	23.005	-18.097	37.141	1.00	39.58	A
	ATOM 5810	OD2	ASP A 110	25.124	-18.429	36.648	1.00	39.67	A
15	ATOM 5811	C	ASP A 110	24.061	-14.977	37.571	1.00	38.89	A
	ATOM 5812	O	ASP A 110	24.802	-13.999	37.663	1.00	38.88	A
	ATOM 5813	N	VAL A 111	23.433	-15.302	36.445	1.00	38.64	A
	ATOM 5814	CA	VAL A 111	23.581	-14.507	35.231	1.00	38.36	A
	ATOM 5815	CB	VAL A 111	23.054	-15.270	34.001	1.00	38.38	A
20	ATOM 5816	CG1	VAL A 111	23.198	-14.412	32.753	1.00	38.34	A
	ATOM 5817	CG2	VAL A 111	23.812	-16.573	33.842	1.00	38.44	A
	ATOM 5818	C	VAL A 111	22.829	-13.183	35.349	1.00	38.10	A
	ATOM 5819	O	VAL A 111	23.297	-12.145	34.880	1.00	37.99	A
	ATOM 5820	N	LYS A 112	21.663	-13.229	35.980	1.00	37.84	A
25	ATOM 5821	CA	LYS A 112	20.851	-12.036	36.163	1.00	37.63	A

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	ATOM 5822	CB	LYS A 112	19.477	-12.414	36.719	1.00	37.62	A
	ATOM 5823	CG	LYS A 112	18.545	-11.233	36.904	1.00	37.60	A
	ATOM 5824	CD	LYS A 112	17.185	-11.663	37.410	1.00	37.64	A
	ATOM 5825	CE	LYS A 112	16.284	-10.457	37.615	1.00	37.70	A
5	ATOM 5826	NZ	LYS A 112	14.951	-10.845	38.142	1.00	37.88	A
	ATOM 5827	C	LYS A 112	21.538	-11.050	37.105	1.00	37.48	A
	ATOM 5828	O	LYS A 112	21.554	-9.846	36.850	1.00	37.36	A
	ATOM 5829	N	GLU A 113	22.112	-11.565	38.189	1.00	37.26	A
	ATOM 5830	CA	GLU A 113	22.796	-10.723	39.166	1.00	37.10	A
10	ATOM 5831	CB	GLU A 113	23.143	-11.537	40.420	1.00	37.36	A
	ATOM 5832	CG	GLU A 113	23.579	-10.692	41.622	1.00	37.69	A
	ATOM 5833	CD	GLU A 113	22.449	-9.851	42.207	1.00	37.86	A
	ATOM 5834	OE1	GLU A 113	22.711	-9.076	43.157	1.00	37.95	A
	ATOM 5835	OE2	GLU A 113	21.301	-9.970	41.723	1.00	37.89	A
15	ATOM 5836	C	GLU A 113	24.070	-10.117	38.573	1.00	36.80	A
	ATOM 5837	O	GLU A 113	24.378	-8.949	38.808	1.00	36.69	A
	ATOM 5838	N	GLN A 114	24.804	-10.914	37.803	1.00	36.47	A
	ATOM 5839	CA	GLN A 114	26.037	-10.448	37.181	1.00	36.17	A
	ATOM 5840	CB	GLN A 114	26.775	-11.622	36.527	1.00	36.48	A
20	ATOM 5841	CG	GLN A 114	27.387	-12.597	37.525	1.00	37.03	A
	ATOM 5842	CD	GLN A 114	27.971	-13.841	36.869	1.00	37.38	A
	ATOM 5843	OE1	GLN A 114	28.847	-13.752	36.005	1.00	37.53	A
	ATOM 5844	NE2	GLN A 114	27.487	-15.012	37.282	1.00	37.45	A
	ATOM 5845	C	GLN A 114	25.768	-9.359	36.148	1.00	35.76	A
25	ATOM 5846	O	GLN A 114	26.582	-8.452	35.963	1.00	35.71	A

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	ATOM 5847	N	MET A 115	24.622	-9.447	35.481	1.00	35.26	A
	ATOM 5848	CA	MET A 115	24.253	-8.459	34.474	1.00	34.74	A
	ATOM 5849	CB	MET A 115	23.147	-9.006	33.573	1.00	35.14	A
	ATOM 5850	CG	MET A 115	22.929	-8.183	32.322	1.00	35.72	A
5	ATOM 5851	SD	MET A 115	24.425	-8.101	31.312	1.00	36.85	A
	ATOM 5852	CE	MET A 115	25.020	-6.470	31.691	1.00	36.19	A
	ATOM 5853	C	MET A 115	23.792	-7.164	35.137	1.00	34.07	A
	ATOM 5854	O	MET A 115	24.214	-6.079	34.745	1.00	34.00	A
	ATOM 5855	N	PHE A 116	22.926	-7.280	36.140	1.00	33.41	A
10	ATOM 5856	CA	PHE A 116	22.437	-6.104	36.856	1.00	32.72	A
	ATOM 5857	CB	PHE A 116	21.485	-6.507	37.982	1.00	32.41	A
	ATOM 5858	CG	PHE A 116	20.039	-6.520	37.583	1.00	32.03	A
	ATOM 5859	CD1	PHE A 116	19.574	-7.415	36.627	1.00	31.76	A
	ATOM 5860	CD2	PHE A 116	19.140	-5.630	38.164	1.00	31.87	A
15	ATOM 5861	CE1	PHE A 116	18.235	-7.426	36.257	1.00	31.75	A
	ATOM 5862	CE2	PHE A 116	17.798	-5.632	37.801	1.00	31.79	A
	ATOM 5863	CZ	PHE A 116	17.343	-6.532	36.845	1.00	31.63	A
	ATOM 5864	C	PHE A 116	23.618	-5.353	37.452	1.00	32.46	A
	ATOM 5865	O	PHE A 116	23.775	-4.147	37.253	1.00	32.41	A
20	ATOM 6152	N	TYR A 152	9.234	10.144	32.617	1.00	9.71	A
	ATOM 6153	CA	TYR A 152	9.916	8.878	32.397	1.00	9.80	A
	ATOM 6154	CB	TYR A 152	10.132	8.650	30.901	1.00	9.99	A
	ATOM 6155	CG	TYR A 152	10.202	7.183	30.526	1.00	10.38	A
	ATOM 6156	CD1	TYR A 152	9.213	6.281	30.944	1.00	10.55	A
25	ATOM 6157	CE1	TYR A 152	9.267	4.928	30.581	1.00	10.77	A

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	ATOM 6158	CD2	TYR	A	152	11.243	6.698	29.742	1.00	10.42	A
	ATOM 6159	CE2	TYR	A	152	11.308	5.353	29.375	1.00	10.66	A
	ATOM 6160	CZ	TYR	A	152	10.325	4.477	29.792	1.00	10.74	A
	ATOM 6161	OH	TYR	A	152	10.393	3.156	29.410	1.00	10.82	A
5	ATOM 6162	C	TYR	A	152	11.245	8.820	33.157	1.00	9.88	A
	ATOM 6163	O	TYR	A	152	11.655	7.755	33.621	1.00	9.73	A
	ATOM 6164	N	TRP	A	153	11.907	9.965	33.296	1.00	9.89	A
	ATOM 6165	CA	TRP	A	153	13.158	10.012	34.036	1.00	10.03	A
	ATOM 6166	CB	TRP	A	153	13.808	11.398	33.925	1.00	10.21	A
10	ATOM 6167	CG	TRP	A	153	14.774	11.688	35.031	1.00	10.40	A
	ATOM 6168	CD2	TRP	A	153	15.930	10.920	35.389	1.00	10.68	A
	ATOM 6169	CE2	TRP	A	153	16.491	11.521	36.539	1.00	10.78	A
	ATOM 6170	CE3	TRP	A	153	16.544	9.783	34.853	1.00	10.67	A
	ATOM 6171	CD1	TRP	A	153	14.688	12.696	35.943	1.00	10.44	A
15	ATOM 6172	NE1	TRP	A	153	15.714	12.603	36.854	1.00	10.64	A
	ATOM 6173	CZ2	TRP	A	153	17.637	11.018	37.167	1.00	10.84	A
	ATOM 6174	CZ3	TRP	A	153	17.689	9.282	35.478	1.00	10.82	A
	ATOM 6175	CH2	TRP	A	153	18.220	9.902	36.623	1.00	10.64	A
	ATOM 6176	C	TRP	A	153	12.893	9.676	35.502	1.00	10.03	A
20	ATOM 6177	O	TRP	A	153	13.602	8.861	36.098	1.00	10.17	A
	ATOM 6178	N	GLU	A	154	11.869	10.295	36.078	1.00	10.10	A
	ATOM 6179	CA	GLU	A	154	11.524	10.048	37.474	1.00	10.17	A
	ATOM 6180	CB	GLU	A	154	10.403	11.001	37.919	1.00	10.10	A
	ATOM 6181	CG	GLU	A	154	10.138	11.016	39.422	1.00	9.74	A
25	ATOM 6182	CD	GLU	A	154	9.268	9.858	39.879	1.00	9.86	A

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	ATOM 6183	OE1	GLU	A	154	9.252	9.560	41.095	1.00	9.89	A
	ATOM 6184	OE2	GLU	A	154	8.588	9.247	39.027	1.00	9.57	A
	ATOM 6185	C	GLU	A	154	11.095	8.587	37.641	1.00	10.51	A
	ATOM 6186	O	GLU	A	154	11.481	7.927	38.608	1.00	10.53	A
5	ATOM 6187	N	ILE	A	155	10.321	8.079	36.683	1.00	10.63	A
	ATOM 6188	CA	ILE	A	155	9.855	6.700	36.739	1.00	10.71	A
	ATOM 6189	CB	ILE	A	155	8.823	6.430	35.625	1.00	10.90	A
	ATOM 6190	CG2	ILE	A	155	8.485	4.944	35.555	1.00	10.77	A
	ATOM 6191	CG1	ILE	A	155	7.559	7.254	35.908	1.00	10.69	A
10	ATOM 6192	CD1	ILE	A	155	6.531	7.198	34.810	1.00	10.76	A
	ATOM 6193	C	ILE	A	155	11.013	5.710	36.641	1.00	10.99	A
	ATOM 6194	O	ILE	A	155	11.147	4.802	37.475	1.00	10.97	A
	ATOM 6195	N	CYS	A	156	11.863	5.902	35.638	1.00	11.08	A
	ATOM 6196	CA	CYS	A	156	13.017	5.030	35.434	1.00	11.24	A
15	ATOM 6197	CB	CYS	A	156	13.719	5.390	34.120	1.00	11.05	A
	ATOM 6198	SG	CYS	A	156	12.789	4.896	32.650	1.00	11.30	A
	ATOM 6199	C	CYS	A	156	14.018	5.108	36.583	1.00	11.50	A
	ATOM 6200	O	CYS	A	156	14.495	4.078	37.065	1.00	11.70	A
	ATOM 6201	N	SER	A	157	14.334	6.325	37.019	1.00	11.70	A
20	ATOM 6202	CA	SER	A	157	15.289	6.512	38.105	1.00	12.05	A
	ATOM 6203	CB	SER	A	157	15.615	7.997	38.287	1.00	11.74	A
	ATOM 6204	OG	SER	A	157	14.494	8.732	38.739	1.00	11.48	A
	ATOM 6205	C	SER	A	157	14.789	5.924	39.424	1.00	12.41	A
	ATOM 6206	O	SER	A	157	15.585	5.500	40.266	1.00	12.70	A
25	ATOM 6207	N	THR	A	158	13.475	5.905	39.612	1.00	12.70	A

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	ATOM 6208	CA	THR A 158	12.913	5.341	40.829	1.00	13.05	A
	ATOM 6209	CB	THR A 158	11.379	5.466	40.853	1.00	13.03	A
	ATOM 6210	OG1	THR A 158	11.014	6.842	41.007	1.00	12.82	A
	ATOM 6211	CG2	THR A 158	10.791	4.659	42.011	1.00	12.99	A
5	ATOM 6212	C	THR A 158	13.284	3.863	40.939	1.00	13.54	A
	ATOM 6213	O	THR A 158	13.754	3.407	41.981	1.00	13.26	A
	ATOM 6214	N	THR A 159	13.068	3.113	39.863	1.00	14.14	A
	ATOM 6215	CA	THR A 159	13.397	1.694	39.872	1.00	14.95	A
	ATOM 6216	CB	THR A 159	12.878	0.995	38.597	1.00	15.00	A
10	ATOM 6217	OG1	THR A 159	11.445	1.015	38.607	1.00	15.26	A
	ATOM 6218	CG2	THR A 159	13.356	-0.459	38.537	1.00	15.00	A
	ATOM 6219	C	THR A 159	14.901	1.459	40.021	1.00	15.25	A
	ATOM 6220	O	THR A 159	15.324	0.580	40.775	1.00	15.54	A
	ATOM 6221	N	LEU A 160	15.709	2.249	39.323	1.00	15.71	A
15	ATOM 6222	CA	LEU A 160	17.158	2.105	39.410	1.00	16.22	A
	ATOM 6223	CB	LEU A 160	17.851	3.066	38.437	1.00	16.17	A
	ATOM 6224	CG	LEU A 160	17.681	2.778	36.940	1.00	16.23	A
	ATOM 6225	CD1	LEU A 160	18.193	3.966	36.137	1.00	16.43	A
	ATOM 6226	CD2	LEU A 160	18.413	1.502	36.548	1.00	15.89	A
20	ATOM 6227	C	LEU A 160	17.653	2.366	40.831	1.00	16.63	A
	ATOM 6228	O	LEU A 160	18.557	1.683	41.316	1.00	16.60	A
	ATOM 6229	N	LEU A 161	17.059	3.356	41.493	1.00	16.97	A
	ATOM 6230	CA	LEU A 161	17.445	3.695	42.858	1.00	17.42	A
	ATOM 6231	CB	LEU A 161	16.733	4.972	43.316	1.00	16.98	A
25	ATOM 6232	CG	LEU A 161	17.249	6.288	42.728	1.00	16.98	A

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	ATOM 6233	CD1	LEU A 161	16.334	7.429	43.147	1.00	16.61	A
	ATOM 6234	CD2	LEU A 161	18.682	6.546	43.201	1.00	16.65	A
	ATOM 6235	C	LEU A 161	17.132	2.548	43.818	1.00	17.85	A
	ATOM 6236	O	LEU A 161	17.722	2.449	44.895	1.00	18.15	A
5	ATOM 6237	N	VAL A 162	16.196	1.691	43.428	1.00	17.99	A
	ATOM 6238	CA	VAL A 162	15.831	0.548	44.245	1.00	18.31	A
	ATOM 6239	CB	VAL A 162	14.611	-0.199	43.647	1.00	18.37	A
	ATOM 6240	CG1	VAL A 162	14.406	-1.530	44.354	1.00	18.47	A
	ATOM 6241	CG2	VAL A 162	13.356	0.660	43.788	1.00	18.42	A
10	ATOM 6242	C	VAL A 162	17.015	-0.418	44.340	1.00	18.61	A
	ATOM 6243	O	VAL A 162	17.236	-1.048	45.378	1.00	18.71	A
	ATOM 6244	N	PHE A 163	17.781	-0.520	43.257	1.00	18.71	A
	ATOM 6245	CA	PHE A 163	18.938	-1.409	43.209	1.00	18.91	A
	ATOM 6246	CB	PHE A 163	18.999	-2.128	41.852	1.00	18.88	A
15	ATOM 6247	CG	PHE A 163	17.789	-2.965	41.558	1.00	18.73	A
	ATOM 6248	CD1	PHE A 163	16.734	-2.448	40.822	1.00	18.63	A
	ATOM 6249	CD2	PHE A 163	17.678	-4.254	42.067	1.00	18.63	A
	ATOM 6250	CE1	PHE A 163	15.584	-3.198	40.599	1.00	18.60	A
	ATOM 6251	CE2	PHE A 163	16.529	-5.011	41.847	1.00	18.56	A
20	ATOM 6252	CZ	PHE A 163	15.483	-4.480	41.114	1.00	18.40	A
	ATOM 6253	C	PHE A 163	20.262	-0.692	43.468	1.00	19.04	A
	ATOM 6254	O	PHE A 163	21.251	-1.326	43.832	1.00	18.99	A
	ATOM 6528	N	THR A 197	4.484	-1.111	45.252	1.00	22.77	A
	ATOM 6529	CA	THR A 197	5.126	-2.297	44.695	1.00	22.69	A
25	ATOM 6530	CB	THR A 197	4.568	-2.649	43.296	1.00	22.64	A

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	ATOM 6531	OG1 THR A 197	4.713	-1.524	42.419	1.00	22.39	A
	ATOM 6532	CG2 THR A 197	3.096	-3.040	43.393	1.00	22.49	A
	ATOM 6533	C THR A 197	6.627	-2.062	44.583	1.00	22.75	A
	ATOM 6534	O THR A 197	7.087	-0.922	44.636	1.00	22.48	A
5	ATOM 6535	N LYS A 198	7.390	-3.139	44.428	1.00	22.84	A
	ATOM 6536	CA LYS A 198	8.835	-3.014	44.305	1.00	23.15	A
	ATOM 6537	CB LYS A 198	9.503	-4.385	44.446	1.00	23.45	A
	ATOM 6538	CG LYS A 198	11.027	-4.339	44.481	1.00	23.89	A
	ATOM 6539	CD LYS A 198	11.617	-5.719	44.748	1.00	24.34	A
10	ATOM 6540	CE LYS A 198	13.135	-5.669	44.905	1.00	24.64	A
	ATOM 6541	NZ LYS A 198	13.715	-7.011	45.224	1.00	24.86	A
	ATOM 6542	C LYS A 198	9.201	-2.391	42.960	1.00	23.13	A
	ATOM 6543	O LYS A 198	9.917	-1.393	42.909	1.00	23.17	A
	ATOM 6544	N LEU A 199	8.706	-2.980	41.876	1.00	23.24	A
15	ATOM 6545	CA LEU A 199	8.989	-2.475	40.537	1.00	23.52	A
	ATOM 6546	CB LEU A 199	9.571	-3.588	39.652	1.00	23.79	A
	ATOM 6547	CG LEU A 199	10.941	-4.180	40.010	1.00	24.11	A
	ATOM 6548	CD1 LEU A 199	11.934	-3.056	40.302	1.00	24.28	A
	ATOM 6549	CD2 LEU A 199	10.810	-5.078	41.220	1.00	24.55	A
20	ATOM 6550	C LEU A 199	7.739	-1.894	39.871	1.00	23.53	A
	ATOM 6551	O LEU A 199	6.704	-1.767	40.557	1.00	23.60	A
	ATOM 6552	OXT LEU A 199	7.807	-1.566	38.669	1.00	23.55	A
	ATOM 6688	N1 GSH H 200	8.305	-2.844	24.998	1.00	20.97	H
	ATOM 6689	CA1 GSH H 200	6.911	-3.081	25.371	1.00	20.94	H
25	ATOM 6690	C1 GSH H 200	6.240	-1.805	25.930	1.00	20.69	H

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	ATOM 6691	O11	GSH	H	200	6.937	-0.824	26.213	1.00	20.48	H
	ATOM 6692	O12	GSH	H	200	4.943	-1.894	26.178	1.00	20.60	H
	ATOM 6693	CB1	GSH	H	200	6.878	-4.158	26.465	1.00	21.02	H
	ATOM 6694	CG1	GSH	H	200	7.003	-5.588	25.927	1.00	21.34	H
5	ATOM 6695	CD1	GSH	H	200	7.105	-6.535	27.153	1.00	21.26	H
	ATOM 6696	OE1	GSH	H	200	7.995	-7.376	27.180	1.00	21.54	H
	ATOM 6697	N2	GSH	H	200	6.151	-6.418	28.106	1.00	21.27	H
	ATOM 6698	CA2	GSH	H	200	6.171	-7.317	29.280	1.00	21.32	H
	ATOM 6699	C2	GSH	H	200	5.234	-8.508	29.053	1.00	21.45	H
10	ATOM 6700	O2	GSH	H	200	4.092	-8.371	28.603	1.00	21.33	H
	ATOM 6701	CB2	GSH	H	200	5.676	-6.608	30.562	1.00	21.16	H
	ATOM 6702	SG2	GSH	H	200	6.895	-5.457	31.266	1.00	20.43	H
	ATOM 6703	N3	GSH	H	200	5.687	-9.697	29.521	1.00	21.62	H
	ATOM 6704	CA3	GSH	H	200	4.848	-10.902	29.598	1.00	21.77	H
15	ATOM 6705	C3	GSH	H	200	5.235	-11.857	28.486	1.00	22.03	H
	ATOM 6706	O31	GSH	H	200	4.505	-12.857	28.339	1.00	22.01	H
	ATOM 6707	O32	GSH	H	200	6.217	-11.556	27.749	1.00	22.31	H
	ATOM 6708	C1	U46	X	201	10.418	-9.029	32.023	1.00	34.62	X
	ATOM 6709	C2	U46	X	201	9.663	-10.080	32.823	1.00	34.77	X
20	ATOM 6710	C3	U46	X	201	9.043	-9.215	33.968	1.00	34.58	X
	ATOM 6711	C4	U46	X	201	8.603	-7.944	33.186	1.00	34.52	X
	ATOM 6712	C5	U46	X	201	9.105	-8.297	31.751	1.00	34.55	X
	ATOM 6713	O6	U46	X	201	8.305	-9.318	31.150	1.00	34.69	X
	ATOM 6714	C7	U46	X	201	8.626	-10.560	31.780	1.00	34.71	X
25	ATOM 6715	C14	U46	X	201	9.215	-6.627	33.663	1.00	33.95	X

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	ATOM 6716	C16	U46	X	201	8.636	-5.646	34.388	1.00	33.42	X
	ATOM 6717	C18	U46	X	201	9.270	-4.351	34.859	1.00	33.17	X
	ATOM 6718	C20	U46	X	201	9.952	-3.549	33.738	1.00	33.13	X
	ATOM 6719	C21	U46	X	201	10.163	-2.068	34.122	1.00	33.29	X
5	ATOM 6720	C24	U46	X	201	10.959	-1.283	33.062	1.00	33.44	X
	ATOM 6721	C27	U46	X	201	10.626	0.219	33.069	1.00	33.39	X
	ATOM 6722	C30	U46	X	201	10.896	0.871	31.709	1.00	33.48	X
	ATOM 6723	O36	U46	X	201	10.227	-4.658	35.841	1.00	33.24	X
	ATOM 6724	C39	U46	X	201	7.877	-9.902	34.751	1.00	34.95	X
10	ATOM 6725	C41	U46	X	201	8.032	-9.785	36.257	1.00	35.34	X
	ATOM 6726	C44	U46	X	201	8.610	-10.654	37.130	1.00	35.62	X
	ATOM 6727	C46	U46	X	201	9.261	-11.994	36.823	1.00	35.69	X
	ATOM 6728	C48	U46	X	201	10.726	-12.086	37.288	1.00	35.70	X
	ATOM 6729	C51	U46	X	201	11.026	-13.433	37.990	1.00	35.67	X
15	ATOM 6730	C54	U46	X	201	12.522	-13.820	37.936	1.00	35.71	X
	ATOM 6731	O57	U46	X	201	12.742	-14.998	38.563	1.00	35.58	X
	ATOM 6732	O58	U46	X	201	13.394	-13.172	37.412	1.00	35.68	X
	ATOM 6734	CA+2	CA2	M	902	12.234	1.221	22.856	1.00	26.18	M
	ATOM 6797	OH2	WAT	S	66	8.810	-7.551	20.104	1.00	14.22	S
20	ATOM 6798	OH2	WAT	S	67	10.805	-8.913	21.442	1.00	18.79	S
	ATOM 6799	OH2	WAT	S	68	7.756	-6.308	22.319	1.00	11.88	S
	ATOM 6800	OH2	WAT	S	69	5.816	-8.813	20.585	1.00	16.62	S
	ATOM 6801	OH2	WAT	S	70	5.092	-6.137	21.429	1.00	8.34	S
	ATOM 6802	OH2	WAT	S	71	5.256	-11.109	19.213	1.00	14.67	S
25	ATOM 6803	OH2	WAT	S	72	3.023	-5.015	22.562	1.00	5.39	S

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	ATOM 6804	OH2 WAT S	73	0.826	-6.659	23.058	1.00	10.24	S
	ATOM 6805	OH2 WAT S	74	2.776	-3.513	24.834	1.00	13.89	S
	ATOM 6806	OH2 WAT S	75	11.519	-4.838	25.573	1.00	37.60	S
	ATOM 6807	OH2 WAT S	76	8.072	-9.994	27.106	1.00	23.21	S
5	ATOM 6808	OH2 WAT S	77	17.600	-2.336	25.194	1.00	29.44	S
	ATOM 6955	OH2 WAT S	228	-2.665	-1.375	34.872	1.00	12.13	S
	ATOM 6956	OH2 WAT S	229	0.635	-8.538	38.751	1.00	19.36	S
	ATOM 6957	OH2 WAT S	230	9.165	-7.382	41.775	1.00	33.05	S
	ATOM 6958	OH2 WAT S	231	1.469	2.057	40.259	1.00	10.55	S
10	ATOM 6959	OH2 WAT S	232	2.424	-0.150	41.673	1.00	7.92	S
	ATOM 6960	OH2 WAT S	233	4.681	1.576	43.702	1.00	20.75	S
	ATOM 6961	OH2 WAT S	234	9.069	3.394	38.480	1.00	10.13	S
	ATOM 6962	OH2 WAT S	235	8.873	1.530	36.291	1.00	19.33	S
	ATOM 6963	OH2 WAT S	236	9.962	-0.719	37.350	1.00	9.21	S
15	ATOM 6964	OH2 WAT S	237	6.538	3.283	32.602	1.00	4.33	S
	ATOM 6966	OH2 WAT S	239	6.866	-5.224	41.878	1.00	15.47	S
	ATOM 7098	OH2 WAT S	376	-2.658	-5.119	20.477	1.00	32.13	S
	ATOM 7100	OH2 WAT S	378	9.041	5.776	21.830	1.00	29.33	S
	ATOM 7101	OH2 WAT S	379	16.468	-6.279	25.400	1.00	37.77	S
20	ATOM 7102	OH2 WAT S	380	11.532	-7.763	23.742	1.00	26.56	S
	ATOM 7103	OH2 WAT S	381	20.121	-7.464	24.596	1.00	31.37	S
	ATOM 7206	OH2 WAT S	487	-6.959	-2.973	28.857	1.00	26.99	S
	ATOM 7220	OH2 WAT S	502	19.741	-12.637	30.102	1.00	30.06	S
	ATOM 7228	OH2 WAT S	511	10.932	3.058	22.095	1.00	23.73	S
25	ATOM 7252	OH2 WAT S	537	14.068	2.624	22.159	1.00	17.19	S

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	ATOM 7253	OH2 WAT S 538	10.354	-0.297	22.259	1.00	23.05	S
	ATOM 7254	OH2 WAT S 539	14.359	0.199	23.830	1.00	17.88	S
	ATOM 7255	OH2 WAT S 540	13.565	-1.416	21.690	1.00	21.98	S
	ATOM 7256	OH2 WAT S 541	14.359	-2.488	23.994	1.00	24.68	S
5	ATOM 7257	OH2 WAT S 542	6.700	1.457	23.387	1.00	7.45	S
	ATOM 7260	OH2 WAT S 545	6.810	4.437	20.115	1.00	9.33	S
	ATOM 7262	OH2 WAT S 548	7.372	2.188	29.676	1.00	13.81	S
	ATOM 7263	OH2 WAT S 551	12.593	1.210	20.664	1.00	23.28	S
	ATOM 7279	OH2 WAT S 568	9.152	-7.664	24.541	1.00	28.73	S
10	ATOM 7330	OH2 WAT S 621	-0.052	-8.417	43.049	1.00	41.72	S
	ATOM 7331	OH2 WAT S 622	4.610	-6.488	42.101	1.00	39.75	S
	ATOM 7334	OH2 WAT S 625	-5.505	-11.363	37.210	1.00	32.13	S
	ATOM 7365	OH2 WAT S 659	12.799	-12.693	21.817	1.00	29.74	S
	ATOM 7419	OH2 WAT S 719	3.738	-8.441	39.590	1.00	44.76	S
15	ATOM 7420	OH2 WAT S 720	-3.644	-7.487	40.846	1.00	28.21	S
	ATOM 7421	OH2 WAT S 721	9.250	0.354	24.552	1.00	31.35	S
	ATOM 7469	OH2 WAT S 779	13.344	-12.993	24.338	1.00	33.74	S
	ATOM 7478	OH2 WAT S 797	9.999	-4.902	29.944	1.00	42.20	S

20 Table 4

Three-dimensional structural coordinate of the complex of human hematopoietic PGDS with magnesium, glutathione and 9,11-dideoxy -9 α , 11 α -methanoepoxyprostaglandine F_{2 α} (U46)

25 ATOM 4966 N TYR A 8 52.373 40.696 69.223 1.00 5.08 A

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	ATOM 4967	CA	TYR	A	8	50.981	40.835	69.625	1.00	5.19	A
	ATOM 4968	CB	TYR	A	8	50.387	42.136	69.066	1.00	5.85	A
	ATOM 4969	CG	TYR	A	8	49.055	42.515	69.678	1.00	5.32	A
	ATOM 4970	CD1	TYR	A	8	48.943	42.758	71.047	1.00	5.34	A
5	ATOM 4971	CE1	TYR	A	8	47.727	43.124	71.619	1.00	5.53	A
	ATOM 4972	CD2	TYR	A	8	47.908	42.646	68.889	1.00	5.77	A
	ATOM 4973	CE2	TYR	A	8	46.685	43.014	69.451	1.00	5.46	A
	ATOM 4974	CZ	TYR	A	8	46.604	43.251	70.815	1.00	5.16	A
	ATOM 4975	OH	TYR	A	8	45.399	43.630	71.365	1.00	5.90	A
10	ATOM 4976	C	TYR	A	8	50.221	39.643	69.062	1.00	5.81	A
	ATOM 4977	O	TYR	A	8	50.803	38.783	68.405	1.00	6.16	A
	ATOM 4978	N	PHE	A	9	48.928	39.581	69.347	1.00	6.65	A
	ATOM 4979	CA	PHE	A	9	48.090	38.518	68.812	1.00	7.22	A
	ATOM 4980	CB	PHE	A	9	46.752	38.461	69.556	1.00	10.27	A
15	ATOM 4981	CG	PHE	A	9	46.868	38.040	70.993	1.00	10.70	A
	ATOM 4982	CD1	PHE	A	9	46.584	38.935	72.021	1.00	13.85	A
	ATOM 4983	CD2	PHE	A	9	47.254	36.744	71.320	1.00	12.21	A
	ATOM 4984	CE1	PHE	A	9	46.683	38.540	73.355	1.00	15.04	A
	ATOM 4985	CE2	PHE	A	9	47.356	36.343	72.650	1.00	13.46	A
20	ATOM 4986	CZ	PHE	A	9	47.070	37.242	73.668	1.00	14.40	A
	ATOM 4987	C	PHE	A	9	47.811	38.860	67.350	1.00	6.45	A
	ATOM 4988	O	PHE	A	9	48.173	39.943	66.873	1.00	6.51	A
	ATOM 4989	N	ASN	A	10	47.178	37.938	66.632	1.00	7.20	A
	ATOM 4990	CA	ASN	A	10	46.822	38.209	65.248	1.00	7.50	A
25	ATOM 4991	CB	ASN	A	10	46.676	36.915	64.445	1.00	8.81	A

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	ATOM 4992	CG	ASN	A	10	46.265	37.172	63.010	1.00	10.65	A
	ATOM 4993	OD1	ASN	A	10	46.628	38.191	62.423	1.00	9.77	A
	ATOM 4994	ND2	ASN	A	10	45.515	36.240	62.430	1.00	12.72	A
	ATOM 4995	C	ASN	A	10	45.489	38.952	65.305	1.00	7.31	A
5	ATOM 4996	O	ASN	A	10	44.425	38.386	65.058	1.00	7.42	A
	ATOM 4997	N	MET	A	11	45.573	40.228	65.668	1.00	6.93	A
	ATOM 4998	CA	MET	A	11	44.424	41.120	65.791	1.00	6.61	A
	ATOM 4999	CB	MET	A	11	43.816	41.082	67.202	1.00	9.76	A
	ATOM 5000	CG	MET	A	11	43.251	39.768	67.703	1.00	12.58	A
10	ATOM 5001	SD	MET	A	11	42.429	40.034	69.312	1.00	16.46	A
	ATOM 5002	CE	MET	A	11	43.822	40.416	70.355	1.00	18.60	A
	ATOM 5003	C	MET	A	11	44.958	42.529	65.612	1.00	4.89	A
	ATOM 5004	O	MET	A	11	46.165	42.765	65.730	1.00	5.10	A
	ATOM 5005	N	ARG	A	12	44.065	43.471	65.333	1.00	4.88	A
15	ATOM 5006	CA	ARG	A	12	44.481	44.863	65.248	1.00	4.58	A
	ATOM 5007	CB	ARG	A	12	43.377	45.722	64.630	1.00	4.90	A
	ATOM 5008	CG	ARG	A	12	43.101	45.396	63.166	1.00	4.93	A
	ATOM 5009	CD	ARG	A	12	42.125	46.404	62.550	1.00	5.92	A
	ATOM 5010	NE	ARG	A	12	40.874	46.486	63.301	1.00	5.59	A
20	ATOM 5011	CZ	ARG	A	12	39.925	45.558	63.273	1.00	6.68	A
	ATOM 5012	NH1	ARG	A	12	40.073	44.477	62.519	1.00	6.84	A
	ATOM 5013	NH2	ARG	A	12	38.841	45.699	64.025	1.00	7.34	A
	ATOM 5014	C	ARG	A	12	44.716	45.251	66.711	1.00	4.87	A
	ATOM 5015	O	ARG	A	12	45.835	45.568	67.112	1.00	5.24	A
25	ATOM 5016	N	GLY	A	13	43.647	45.193	67.500	1.00	5.06	A

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	ATOM 5017	CA	GLY	A	13	43.722	45.495	68.916	1.00	4.83	A
	ATOM 5018	C	GLY	A	13	44.620	46.641	69.327	1.00	4.65	A
	ATOM 5019	O	GLY	A	13	44.611	47.717	68.718	1.00	5.04	A
	ATOM 5020	N	ARG	A	14	45.404	46.397	70.373	1.00	4.18	A
5	ATOM 5021	CA	ARG	A	14	46.305	47.398	70.929	1.00	5.36	A
	ATOM 5022	CB	ARG	A	14	46.573	47.085	72.401	1.00	5.09	A
	ATOM 5023	CG	ARG	A	14	45.315	47.228	73.252	1.00	5.96	A
	ATOM 5024	CD	ARG	A	14	45.594	46.965	74.727	1.00	8.03	A
	ATOM 5025	NE	ARG	A	14	44.524	47.502	75.570	1.00	10.77	A
10	ATOM 5026	CZ	ARG	A	14	43.670	46.772	76.281	1.00	12.04	A
	ATOM 5027	NH1	ARG	A	14	43.742	45.449	76.268	1.00	13.88	A
	ATOM 5028	NH2	ARG	A	14	42.740	47.372	77.011	1.00	15.99	A
	ATOM 5029	C	ARG	A	14	47.618	47.571	70.188	1.00	4.92	A
	ATOM 5030	O	ARG	A	14	48.394	48.465	70.509	1.00	6.47	A
15	ATOM 5031	N	ALA	A	15	47.878	46.728	69.199	1.00	4.71	A
	ATOM 5032	CA	ALA	A	15	49.111	46.864	68.439	1.00	4.73	A
	ATOM 5033	CB	ALA	A	15	49.617	45.491	68.020	1.00	7.01	A
	ATOM 5034	C	ALA	A	15	48.907	47.729	67.203	1.00	4.72	A
	ATOM 5035	O	ALA	A	15	49.867	48.277	66.661	1.00	4.50	A
20	ATOM 5036	N	GLU	A	16	47.656	47.882	66.775	1.00	4.21	A
	ATOM 5037	CA	GLU	A	16	47.386	48.606	65.542	1.00	4.17	A
	ATOM 5038	CB	GLU	A	16	45.888	48.555	65.220	1.00	4.19	A
	ATOM 5039	CG	GLU	A	16	45.564	48.801	63.741	1.00	5.10	A
	ATOM 5040	CD	GLU	A	16	46.069	47.700	62.804	1.00	5.24	A
25	ATOM 5041	OE1	GLU	A	16	46.619	46.682	63.283	1.00	5.72	A

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	ATOM 5042	OE2	GLU	A	16	45.907	47.864	61.575	1.00	5.89	A
	ATOM 5043	C	GLU	A	16	47.904	50.034	65.463	1.00	4.67	A
	ATOM 5044	O	GLU	A	16	48.364	50.459	64.404	1.00	4.75	A
	ATOM 5045	N	ILE	A	17	47.859	50.776	66.566	1.00	4.26	A
5	ATOM 5046	CA	ILE	A	17	48.351	52.146	66.529	1.00	4.04	A
	ATOM 5047	CB	ILE	A	17	48.092	52.876	67.889	1.00	5.08	A
	ATOM 5048	CG2	ILE	A	17	48.797	52.165	69.029	1.00	5.12	A
	ATOM 5049	CG1	ILE	A	17	48.539	54.337	67.794	1.00	4.72	A
	ATOM 5050	CD1	ILE	A	17	47.815	55.138	66.720	1.00	6.77	A
10	ATOM 5051	C	ILE	A	17	49.841	52.150	66.158	1.00	4.37	A
	ATOM 5052	O	ILE	A	17	50.301	53.003	65.394	1.00	5.08	A
	ATOM 5242	N	TRP	A	39	50.877	31.481	73.859	1.00	14.53	A
	ATOM 5243	CA	TRP	A	39	50.756	32.520	74.879	1.00	13.46	A
	ATOM 5244	CB	TRP	A	39	49.282	32.747	75.231	1.00	13.58	A
15	ATOM 5245	CG	TRP	A	39	49.060	33.765	76.321	1.00	12.94	A
	ATOM 5246	CD2	TRP	A	39	49.582	35.102	76.384	1.00	12.06	A
	ATOM 5247	CE2	TRP	A	39	49.128	35.671	77.593	1.00	12.15	A
	ATOM 5248	CE3	TRP	A	39	50.392	35.874	75.537	1.00	10.40	A
	ATOM 5249	CD1	TRP	A	39	48.328	33.591	77.460	1.00	13.75	A
20	ATOM 5250	NE1	TRP	A	39	48.365	34.728	78.230	1.00	13.97	A
	ATOM 5251	CZ2	TRP	A	39	49.454	36.974	77.981	1.00	11.46	A
	ATOM 5252	CZ3	TRP	A	39	50.717	37.176	75.926	1.00	10.56	A
	ATOM 5253	CH2	TRP	A	39	50.247	37.709	77.137	1.00	10.60	A
	ATOM 5254	C	TRP	A	39	51.564	32.262	76.156	1.00	14.42	A
25	ATOM 5255	O	TRP	A	39	52.316	33.127	76.592	1.00	13.42	A

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	ATOM 5256	N	PRO A	40	51.424	31.076	76.774	1.00	13.83	A
	ATOM 5257	CD	PRO A	40	50.509	29.950	76.512	1.00	15.37	A
	ATOM 5258	CA	PRO A	40	52.202	30.843	77.995	1.00	13.84	A
	ATOM 5259	CB	PRO A	40	51.885	29.388	78.329	1.00	14.82	A
5	ATOM 5260	CG	PRO A	40	50.467	29.254	77.861	1.00	15.27	A
	ATOM 5261	C	PRO A	40	53.697	31.089	77.809	1.00	14.02	A
	ATOM 5262	O	PRO A	40	54.342	31.712	78.656	1.00	14.68	A
	ATOM 5263	N	GLU A	41	54.245	30.606	76.700	1.00	14.37	A
	ATOM 5264	CA	GLU A	41	55.664	30.784	76.422	1.00	15.32	A
10	ATOM 5265	CB	GLU A	41	56.079	29.953	75.205	1.00	18.64	A
	ATOM 5266	CG	GLU A	41	54.940	29.199	74.548	1.00	25.28	A
	ATOM 5267	CD	GLU A	41	55.423	28.170	73.548	1.00	27.49	A
	ATOM 5268	OE1	GLU A	41	56.616	28.201	73.183	1.00	29.60	A
	ATOM 5269	OE2	GLU A	41	54.608	27.334	73.116	1.00	30.19	A
15	ATOM 5270	C	GLU A	41	56.005	32.253	76.188	1.00	13.50	A
	ATOM 5271	O	GLU A	41	56.988	32.761	76.723	1.00	15.87	A
	ATOM 5272	N	ILE A	42	55.190	32.931	75.388	1.00	12.31	A
	ATOM 5273	CA	ILE A	42	55.413	34.342	75.095	1.00	12.42	A
	ATOM 5274	CB	ILE A	42	54.407	34.852	74.031	1.00	12.64	A
20	ATOM 5275	CG2	ILE A	42	54.485	36.374	73.916	1.00	12.49	A
	ATOM 5276	CG1	ILE A	42	54.697	34.197	72.677	1.00	14.88	A
	ATOM 5277	CD1	ILE A	42	56.018	34.607	72.054	1.00	16.40	A
	ATOM 5278	C	ILE A	42	55.276	35.196	76.358	1.00	10.62	A
	ATOM 5279	O	ILE A	42	56.111	36.063	76.625	1.00	11.25	A
25	ATOM 5280	N	LYS A	43	54.228	34.941	77.131	1.00	11.00	A

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	ATOM 5281	CA	LYS A	43	53.969	35.697	78.351	1.00	10.64	A
	ATOM 5282	CB	LYS A	43	52.722	35.144	79.052	1.00	9.83	A
	ATOM 5283	CG	LYS A	43	52.292	35.936	80.279	1.00	10.83	A
	ATOM 5284	CD	LYS A	43	51.053	35.326	80.910	1.00	12.63	A
5	ATOM 5285	CE	LYS A	43	50.652	36.051	82.183	1.00	14.51	A
	ATOM 5286	NZ	LYS A	43	49.477	35.397	82.820	1.00	14.93	A
	ATOM 5287	C	LYS A	43	55.143	35.703	79.323	1.00	12.13	A
	ATOM 5288	O	LYS A	43	55.384	36.699	80.005	1.00	12.18	A
	ATOM 5328	N	GLY A	49	53.610	40.833	81.753	1.00	7.16	A
10	ATOM 5329	CA	GLY A	49	52.668	39.832	81.287	1.00	8.61	A
	ATOM 5330	C	GLY A	49	51.654	40.290	80.260	1.00	6.93	A
	ATOM 5331	O	GLY A	49	50.653	39.608	80.038	1.00	7.98	A
	ATOM 5332	N	LYS A	50	51.907	41.429	79.619	1.00	6.55	A
	ATOM 5333	CA	LYS A	50	50.976	41.949	78.625	1.00	6.43	A
15	ATOM 5334	CB	LYS A	50	50.305	43.240	79.120	1.00	7.04	A
	ATOM 5335	CG	LYS A	50	49.749	43.196	80.530	1.00	9.59	A
	ATOM 5336	CD	LYS A	50	48.616	42.198	80.672	1.00	11.11	A
	ATOM 5337	CE	LYS A	50	48.089	42.190	82.097	1.00	15.13	A
	ATOM 5338	NZ	LYS A	50	49.205	42.086	83.079	1.00	17.69	A
20	ATOM 5339	C	LYS A	50	51.641	42.272	77.300	1.00	5.28	A
	ATOM 5340	O	LYS A	50	52.846	42.538	77.232	1.00	5.40	A
	ATOM 5341	N	ILE A	51	50.837	42.241	76.247	1.00	4.98	A
	ATOM 5342	CA	ILE A	51	51.300	42.612	74.923	1.00	5.31	A
	ATOM 5343	CB	ILE A	51	51.297	41.414	73.929	1.00	6.08	A
25	ATOM 5344	CG2	ILE A	51	52.577	40.606	74.121	1.00	7.61	A

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	ATOM 5345	CG1	ILE	A	51	50.044	40.552	74.104	1.00	7.83	A
	ATOM 5346	CD1	ILE	A	51	49.971	39.380	73.132	1.00	11.35	A
	ATOM 5347	C	ILE	A	51	50.350	43.716	74.449	1.00	4.83	A
	ATOM 5348	O	ILE	A	51	49.228	43.847	74.929	1.00	5.85	A
5	ATOM 5349	N	PRO	A	52	50.778	44.515	73.461	1.00	4.61	A
	ATOM 5350	CD	PRO	A	52	50.013	45.710	73.057	1.00	4.91	A
	ATOM 5351	CA	PRO	A	52	52.047	44.434	72.746	1.00	4.74	A
	ATOM 5352	CB	PRO	A	52	51.803	45.352	71.556	1.00	5.22	A
	ATOM 5353	CG	PRO	A	52	51.008	46.472	72.190	1.00	6.07	A
10	ATOM 5354	C	PRO	A	52	53.327	44.841	73.456	1.00	5.16	A
	ATOM 5355	O	PRO	A	52	53.326	45.548	74.469	1.00	4.84	A
	ATOM 5356	N	ILE	A	53	54.423	44.329	72.909	1.00	4.77	A
	ATOM 5357	CA	ILE	A	53	55.747	44.742	73.323	1.00	4.63	A
	ATOM 5358	CB	ILE	A	53	56.576	43.680	74.116	1.00	5.58	A
15	ATOM 5359	CG2	ILE	A	53	55.986	43.498	75.498	1.00	6.57	A
	ATOM 5360	CG1	ILE	A	53	56.711	42.376	73.332	1.00	6.10	A
	ATOM 5361	CD1	ILE	A	53	57.853	41.501	73.831	1.00	8.86	A
	ATOM 5362	C	ILE	A	53	56.439	45.024	71.998	1.00	4.92	A
	ATOM 5363	O	ILE	A	53	56.056	44.484	70.951	1.00	4.78	A
20	ATOM 5423	N	HIS	A	62	57.230	48.257	76.387	1.00	5.48	A
	ATOM 5424	CA	HIS	A	62	55.869	47.762	76.529	1.00	5.13	A
	ATOM 5425	CB	HIS	A	62	55.742	46.832	77.744	1.00	5.58	A
	ATOM 5426	CG	HIS	A	62	55.930	47.514	79.060	1.00	4.58	A
	ATOM 5427	CD2	HIS	A	62	57.037	48.000	79.664	1.00	5.33	A
25	ATOM 5428	ND1	HIS	A	62	54.877	47.778	79.911	1.00	5.59	A

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	ATOM 5429	CE1	HIS	A	62	55.333	48.400	80.982	1.00	5.03	A
	ATOM 5430	NE2	HIS	A	62	56.639	48.549	80.860	1.00	6.03	A
	ATOM 5431	C	HIS	A	62	54.925	48.962	76.626	1.00	4.66	A
	ATOM 5432	O	HIS	A	62	55.386	50.105	76.654	1.00	5.51	A
5	ATOM 5433	N	GLN	A	63	53.619	48.684	76.647	1.00	4.29	A
	ATOM 5434	CA	GLN	A	63	52.542	49.684	76.704	1.00	4.47	A
	ATOM 5435	CB	GLN	A	63	52.799	50.722	77.803	1.00	5.14	A
	ATOM 5436	CG	GLN	A	63	52.408	50.230	79.196	1.00	5.62	A
	ATOM 5437	CD	GLN	A	63	50.906	50.052	79.366	1.00	5.35	A
10	ATOM 5438	OE1	GLN	A	63	50.112	50.483	78.523	1.00	4.91	A
	ATOM 5439	NE2	GLN	A	63	50.508	49.434	80.474	1.00	5.54	A
	ATOM 5440	C	GLN	A	63	52.378	50.337	75.335	1.00	4.53	A
	ATOM 5441	O	GLN	A	63	53.197	51.150	74.908	1.00	4.75	A
	ATOM 5442	N	SER	A	64	51.298	49.970	74.652	1.00	4.47	A
15	ATOM 5443	CA	SER	A	64	51.049	50.446	73.299	1.00	5.16	A
	ATOM 5444	CB	SER	A	64	49.693	49.935	72.796	1.00	4.88	A
	ATOM 5445	OG	SER	A	64	48.605	50.551	73.460	1.00	5.68	A
	ATOM 5446	C	SER	A	64	51.149	51.942	73.054	1.00	4.97	A
	ATOM 5447	O	SER	A	64	51.742	52.366	72.062	1.00	5.10	A
20	ATOM 5448	N	LEU	A	65	50.583	52.749	73.943	1.00	4.29	A
	ATOM 5449	CA	LEU	A	65	50.616	54.189	73.744	1.00	4.24	A
	ATOM 5450	CB	LEU	A	65	49.468	54.843	74.514	1.00	5.94	A
	ATOM 5451	CG	LEU	A	65	48.110	54.218	74.171	1.00	6.96	A
	ATOM 5452	CD1	LEU	A	65	47.017	54.953	74.937	1.00	9.08	A
25	ATOM 5453	CD2	LEU	A	65	47.857	54.274	72.666	1.00	8.54	A

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	ATOM 5454	C	LEU A	65	51.962	54.802	74.114	1.00	4.91	A
	ATOM 5455	O	LEU A	65	52.360	55.817	73.544	1.00	5.28	A
	ATOM 5662	N	ASP A	93	44.344	59.210	75.556	1.00	4.56	A
	ATOM 5663	CA	ASP A	93	43.975	58.590	76.829	1.00	4.81	A
5	ATOM 5664	CB	ASP A	93	44.674	59.281	78.008	1.00	5.82	A
	ATOM 5665	CG	ASP A	93	46.052	58.688	78.299	1.00	6.27	A
	ATOM 5666	OD1	ASP A	93	46.654	59.050	79.336	1.00	8.17	A
	ATOM 5667	OD2	ASP A	93	46.534	57.858	77.497	1.00	6.94	A
	ATOM 5668	C	ASP A	93	42.455	58.581	77.031	1.00	4.64	A
10	ATOM 5669	O	ASP A	93	41.914	57.667	77.647	1.00	5.45	A
	ATOM 5670	N	THR A	94	41.760	59.589	76.513	1.00	4.84	A
	ATOM 5671	CA	THR A	94	40.307	59.616	76.642	1.00	5.76	A
	ATOM 5672	CB	THR A	94	39.745	60.972	76.166	1.00	6.34	A
	ATOM 5673	OG1	THR A	94	40.156	61.992	77.086	1.00	7.42	A
15	ATOM 5674	CG2	THR A	94	38.223	60.943	76.110	1.00	8.19	A
	ATOM 5675	C	THR A	94	39.718	58.460	75.825	1.00	6.13	A
	ATOM 5676	O	THR A	94	38.803	57.764	76.276	1.00	6.09	A
	ATOM 5677	N	LEU A	95	40.253	58.247	74.628	1.00	4.62	A
	ATOM 5678	CA	LEU A	95	39.788	57.153	73.785	1.00	5.06	A
20	ATOM 5679	CB	LEU A	95	40.426	57.233	72.400	1.00	5.92	A
	ATOM 5680	CG	LEU A	95	39.966	58.395	71.519	1.00	6.51	A
	ATOM 5681	CD1	LEU A	95	40.809	58.448	70.253	1.00	7.81	A
	ATOM 5682	CD2	LEU A	95	38.495	58.215	71.174	1.00	8.77	A
	ATOM 5683	C	LEU A	95	40.143	55.819	74.423	1.00	4.85	A
25	ATOM 5684	O	LEU A	95	39.321	54.907	74.480	1.00	5.32	A

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	ATOM 5685	N	ASP	A	96	41.373	55.711	74.912	1.00	5.08	A
	ATOM 5686	CA	ASP	A	96	41.830	54.472	75.524	1.00	4.86	A
	ATOM 5687	CB	ASP	A	96	43.328	54.556	75.817	1.00	5.00	A
	ATOM 5688	CG	ASP	A	96	43.975	53.191	75.916	1.00	6.28	A
5	ATOM 5689	OD1	ASP	A	96	43.865	52.415	74.945	1.00	7.24	A
	ATOM 5690	OD2	ASP	A	96	44.593	52.896	76.958	1.00	8.87	A
	ATOM 5691	C	ASP	A	96	41.056	54.146	76.797	1.00	5.03	A
	ATOM 5692	O	ASP	A	96	40.784	52.978	77.082	1.00	5.59	A
	ATOM 5693	N	ASP	A	97	40.702	55.173	77.564	1.00	5.23	A
10	ATOM 5694	CA	ASP	A	97	39.926	54.974	78.784	1.00	5.46	A
	ATOM 5695	CB	ASP	A	97	39.585	56.317	79.436	1.00	6.58	A
	ATOM 5696	CG	ASP	A	97	40.721	56.890	80.261	1.00	6.62	A
	ATOM 5697	OD1	ASP	A	97	40.597	58.061	80.677	1.00	7.17	A
	ATOM 5698	OD2	ASP	A	97	41.721	56.185	80.504	1.00	7.79	A
15	ATOM 5699	C	ASP	A	97	38.621	54.269	78.426	1.00	6.00	A
	ATOM 5700	O	ASP	A	97	38.207	53.322	79.100	1.00	6.84	A
	ATOM 5701	N	PHE	A	98	37.969	54.732	77.364	1.00	5.70	A
	ATOM 5702	CA	PHE	A	98	36.712	54.122	76.964	1.00	5.97	A
	ATOM 5703	CB	PHE	A	98	36.013	54.962	75.898	1.00	6.49	A
20	ATOM 5704	CG	PHE	A	98	34.603	54.532	75.635	1.00	7.36	A
	ATOM 5705	CD1	PHE	A	98	33.662	54.547	76.659	1.00	9.72	A
	ATOM 5706	CD2	PHE	A	98	34.217	54.088	74.379	1.00	7.45	A
	ATOM 5707	CE1	PHE	A	98	32.354	54.123	76.434	1.00	10.12	A
	ATOM 5708	CE2	PHE	A	98	32.911	53.662	74.140	1.00	9.08	A
25	ATOM 5709	CZ	PHE	A	98	31.979	53.680	75.172	1.00	9.33	A

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	ATOM 5710	C	PHE A	98	36.906	52.698	76.452	1.00	6.08	A
	ATOM 5711	O	PHE A	98	36.168	51.789	76.839	1.00	6.41	A
	ATOM 5712	N	MET A	99	37.896	52.490	75.589	1.00	6.17	A
	ATOM 5713	CA	MET A	99	38.146	51.152	75.062	1.00	5.91	A
5	ATOM 5714	CB	MET A	99	39.330	51.155	74.091	1.00	7.58	A
	ATOM 5715	CG	MET A	99	39.159	52.043	72.860	1.00	7.35	A
	ATOM 5716	SD	MET A	99	37.673	51.709	71.886	1.00	7.56	A
	ATOM 5717	CE	MET A	99	38.136	50.177	71.036	1.00	9.56	A
	ATOM 5718	C	MET A	99	38.439	50.178	76.198	1.00	6.10	A
10	ATOM 5719	O	MET A	99	38.060	49.005	76.139	1.00	7.35	A
	ATOM 5720	N	SER A	100	39.108	50.671	77.236	1.00	6.09	A
	ATOM 5721	CA	SER A	100	39.465	49.839	78.382	1.00	8.79	A
	ATOM 5722	CB	SER A	100	40.533	50.546	79.220	1.00	9.54	A
	ATOM 5723	OG	SER A	100	41.722	50.717	78.466	1.00	15.41	A
15	ATOM 5724	C	SER A	100	38.279	49.449	79.266	1.00	9.77	A
	ATOM 5725	O	SER A	100	38.415	48.591	80.142	1.00	12.78	A
	ATOM 5726	N	CYS A	101	37.123	50.067	79.033	1.00	9.75	A
	ATOM 5727	CA	CYS A	101	35.920	49.764	79.808	1.00	11.59	A
	ATOM 5728	CB	CYS A	101	34.892	50.892	79.680	1.00	12.49	A
20	ATOM 5729	SG	CYS A	101	35.263	52.370	80.617	1.00	15.69	A
	ATOM 5730	C	CYS A	101	35.260	48.469	79.351	1.00	10.47	A
	ATOM 5731	O	CYS A	101	34.497	47.857	80.100	1.00	12.82	A
	ATOM 5732	N	PHE A	102	35.542	48.063	78.119	1.00	10.24	A
	ATOM 5733	CA	PHE A	102	34.941	46.855	77.571	1.00	10.36	A
25	ATOM 5734	CB	PHE A	102	35.009	46.877	76.045	1.00	10.28	A

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	ATOM 5735	CG	PHE A	102	34.151	47.936	75.420	1.00	8.84	A
	ATOM 5736	CD1	PHE A	102	34.567	49.263	75.386	1.00	9.33	A
	ATOM 5737	CD2	PHE A	102	32.910	47.609	74.884	1.00	9.36	A
	ATOM 5738	CE1	PHE A	102	33.756	50.251	74.829	1.00	8.74	A
5	ATOM 5739	CE2	PHE A	102	32.092	48.586	74.325	1.00	9.38	A
	ATOM 5740	CZ	PHE A	102	32.516	49.911	74.297	1.00	7.96	A
	ATOM 5741	C	PHE A	102	35.581	45.577	78.097	1.00	11.75	A
	ATOM 5742	O	PHE A	102	36.801	45.487	78.213	1.00	12.38	A
	ATOM 5743	N	PRO A	103	34.755	44.566	78.420	1.00	12.10	A
10	ATOM 5744	CD	PRO A	103	33.282	44.633	78.463	1.00	12.55	A
	ATOM 5745	CA	PRO A	103	35.232	43.278	78.937	1.00	13.72	A
	ATOM 5746	CB	PRO A	103	34.005	42.730	79.650	1.00	14.58	A
	ATOM 5747	CG	PRO A	103	32.898	43.194	78.758	1.00	13.49	A
	ATOM 5748	C	PRO A	103	35.709	42.361	77.815	1.00	14.61	A
15	ATOM 5749	O	PRO A	103	35.101	41.325	77.544	1.00	15.36	A
	ATOM 5750	N	TRP A	104	36.804	42.744	77.171	1.00	14.45	A
	ATOM 5751	CA	TRP A	104	37.352	41.968	76.068	1.00	15.73	A
	ATOM 5752	CB	TRP A	104	38.617	42.634	75.529	1.00	15.71	A
	ATOM 5753	CG	TRP A	104	38.438	44.071	75.158	1.00	13.26	A
20	ATOM 5754	CD2	TRP A	104	37.817	44.572	73.972	1.00	13.03	A
	ATOM 5755	CE2	TRP A	104	37.825	45.981	74.063	1.00	11.27	A
	ATOM 5756	CE3	TRP A	104	37.242	43.965	72.848	1.00	12.96	A
	ATOM 5757	CD1	TRP A	104	38.797	45.163	75.895	1.00	12.87	A
	ATOM 5758	NE1	TRP A	104	38.433	46.315	75.242	1.00	11.57	A
25	ATOM 5759	CZ2	TRP A	104	37.288	46.796	73.060	1.00	13.14	A

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	ATOM 5760	CZ3	TRP	A	104	36.707	44.776	71.853	1.00	13.80	A
	ATOM 5761	CH2	TRP	A	104	36.731	46.176	71.970	1.00	14.33	A
	ATOM 5762	C	TRP	A	104	37.670	40.516	76.424	1.00	17.38	A
	ATOM 5763	O	TRP	A	104	37.534	39.628	75.591	1.00	18.27	A
5	ATOM 5764	N	ALA	A	105	38.088	40.265	77.658	1.00	18.99	A
	ATOM 5765	CA	ALA	A	105	38.443	38.907	78.053	1.00	21.60	A
	ATOM 5766	CB	ALA	A	105	39.670	38.942	78.956	1.00	21.34	A
	ATOM 5767	C	ALA	A	105	37.330	38.111	78.726	1.00	23.19	A
	ATOM 5768	O	ALA	A	105	37.545	36.968	79.130	1.00	23.27	A
10	ATOM 5769	N	GLU	A	106	36.144	38.700	78.843	1.00	24.01	A
	ATOM 5770	CA	GLU	A	106	35.028	38.009	79.480	1.00	25.35	A
	ATOM 5771	CB	GLU	A	106	33.773	38.884	79.457	1.00	25.81	A
	ATOM 5772	CG	GLU	A	106	32.545	38.207	80.053	1.00	26.97	A
	ATOM 5773	CD	GLU	A	106	32.799	37.651	81.443	1.00	27.81	A
15	ATOM 5774	OE1	GLU	A	106	33.119	38.441	82.356	1.00	28.08	A
	ATOM 5775	OE2	GLU	A	106	32.681	36.419	81.620	1.00	28.82	A
	ATOM 5776	C	GLU	A	106	34.735	36.666	78.819	1.00	25.88	A
	ATOM 5777	O	GLU	A	106	34.530	36.582	77.609	1.00	25.18	A
	ATOM 5778	N	LYS	A	107	34.713	35.618	79.637	1.00	27.20	A
20	ATOM 5779	CA	LYS	A	107	34.462	34.255	79.179	1.00	28.80	A
	ATOM 5780	CB	LYS	A	107	34.794	33.252	80.292	1.00	29.93	A
	ATOM 5781	CG	LYS	A	107	36.017	33.600	81.132	1.00	31.92	A
	ATOM 5782	CD	LYS	A	107	35.769	34.840	81.986	1.00	33.29	A
	ATOM 5783	CE	LYS	A	107	36.998	35.235	82.776	1.00	35.16	A
25	ATOM 5784	NZ	LYS	A	107	36.888	36.631	83.286	1.00	36.27	A

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	ATOM 5785	C	LYS A 107	33.000	34.085	78.779	1.00	28.48	A
	ATOM 5786	O	LYS A 107	32.693	33.623	77.681	1.00	29.44	A
	ATOM 5787	N	LYS A 108	32.107	34.456	79.690	1.00	28.29	A
	ATOM 5788	CA	LYS A 108	30.671	34.350	79.462	1.00	28.16	A
5	ATOM 5789	CB	LYS A 108	29.920	34.648	80.761	1.00	29.14	A
	ATOM 5790	CG	LYS A 108	30.297	33.723	81.911	1.00	30.38	A
	ATOM 5791	CD	LYS A 108	29.548	34.069	83.188	1.00	32.02	A
	ATOM 5792	CE	LYS A 108	29.946	35.439	83.720	1.00	33.28	A
	ATOM 5793	NZ	LYS A 108	31.394	35.501	84.063	1.00	34.77	A
10	ATOM 5794	C	LYS A 108	30.227	35.311	78.364	1.00	27.82	A
	ATOM 5795	O	LYS A 108	30.147	36.521	78.576	1.00	26.75	A
	ATOM 5796	N	GLN A 109	29.932	34.759	77.191	1.00	27.48	A
	ATOM 5797	CA	GLN A 109	29.510	35.559	76.046	1.00	27.67	A
	ATOM 5798	CB	GLN A 109	29.326	34.662	74.820	1.00	29.61	A
15	ATOM 5799	CG	GLN A 109	30.615	34.010	74.345	1.00	32.22	A
	ATOM 5800	CD	GLN A 109	31.706	35.024	74.043	1.00	33.48	A
	ATOM 5801	OE1	GLN A 109	31.559	35.869	73.161	1.00	35.21	A
	ATOM 5802	NE2	GLN A 109	32.808	34.943	74.779	1.00	33.63	A
	ATOM 5803	C	GLN A 109	28.238	36.362	76.290	1.00	26.71	A
20	ATOM 5804	O	GLN A 109	28.121	37.497	75.833	1.00	25.25	A
	ATOM 5805	N	ASP A 110	27.284	35.774	77.004	1.00	26.14	A
	ATOM 5806	CA	ASP A 110	26.030	36.459	77.293	1.00	25.81	A
	ATOM 5807	CB	ASP A 110	25.071	35.516	78.031	1.00	28.34	A
	ATOM 5808	CG	ASP A 110	25.701	34.879	79.254	1.00	30.43	A
25	ATOM 5809	OD1	ASP A 110	25.955	35.597	80.242	1.00	31.82	A

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	ATOM 5810	OD2	ASP	A	110	25.945	33.654	79.226	1.00	33.72	A
	ATOM 5811	C	ASP	A	110	26.275	37.722	78.115	1.00	24.06	A
	ATOM 5812	O	ASP	A	110	25.718	38.781	77.823	1.00	23.68	A
	ATOM 5813	N	VAL	A	111	27.117	37.610	79.138	1.00	22.43	A
5	ATOM 5814	CA	VAL	A	111	27.433	38.748	79.994	1.00	20.34	A
	ATOM 5815	CB	VAL	A	111	28.257	38.311	81.226	1.00	21.27	A
	ATOM 5816	CG1	VAL	A	111	28.620	39.523	82.070	1.00	22.02	A
	ATOM 5817	CG2	VAL	A	111	27.464	37.313	82.053	1.00	22.25	A
	ATOM 5818	C	VAL	A	111	28.240	39.778	79.215	1.00	18.84	A
10	ATOM 5819	O	VAL	A	111	28.005	40.980	79.309	1.00	17.77	A
	ATOM 5820	N	LYS	A	112	29.195	39.292	78.442	1.00	17.36	A
	ATOM 5821	CA	LYS	A	112	30.048	40.154	77.650	1.00	16.73	A
	ATOM 5822	CB	LYS	A	112	31.037	39.287	76.919	1.00	17.64	A
	ATOM 5823	CG	LYS	A	112	32.075	40.014	76.182	1.00	18.95	A
15	ATOM 5824	CD	LYS	A	112	32.954	38.942	75.717	1.00	21.64	A
	ATOM 5825	CE	LYS	A	112	34.038	39.471	74.948	1.00	22.51	A
	ATOM 5826	NZ	LYS	A	112	34.561	38.318	74.176	1.00	25.51	A
	ATOM 5827	C	LYS	A	112	29.242	40.977	76.656	1.00	15.52	A
	ATOM 5828	O	LYS	A	112	29.410	42.192	76.550	1.00	13.43	A
20	ATOM 5829	N	GLU	A	113	28.366	40.298	75.925	1.00	14.92	A
	ATOM 5830	CA	GLU	A	113	27.520	40.947	74.938	1.00	15.67	A
	ATOM 5831	CB	GLU	A	113	26.626	39.904	74.271	1.00	18.01	A
	ATOM 5832	CG	GLU	A	113	25.680	40.492	73.263	1.00	23.31	A
	ATOM 5833	CD	GLU	A	113	24.799	39.452	72.598	1.00	25.74	A
25	ATOM 5834	OE1	GLU	A	113	25.338	38.456	72.073	1.00	27.13	A

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	ATOM 5835	OE2	GLU	A	113	23.565	39.642	72.587	1.00	28.97	A
	ATOM 5836	C	GLU	A	113	26.659	42.036	75.575	1.00	14.49	A
	ATOM 5837	O	GLU	A	113	26.556	43.148	75.053	1.00	13.30	A
	ATOM 5838	N	GLN	A	114	26.046	41.709	76.708	1.00	14.04	A
5	ATOM 5839	CA	GLN	A	114	25.196	42.657	77.418	1.00	14.13	A
	ATOM 5840	CB	GLN	A	114	24.622	42.011	78.685	1.00	15.69	A
	ATOM 5841	CG	GLN	A	114	23.799	42.961	79.545	1.00	18.28	A
	ATOM 5842	CD	GLN	A	114	22.512	43.407	78.874	1.00	19.74	A
	ATOM 5843	OE1	GLN	A	114	21.856	44.344	79.330	1.00	23.56	A
10	ATOM 5844	NE2	GLN	A	114	22.140	42.733	77.792	1.00	21.05	A
	ATOM 5845	C	GLN	A	114	25.966	43.920	77.793	1.00	13.10	A
	ATOM 5846	O	GLN	A	114	25.486	45.033	77.583	1.00	12.07	A
	ATOM 5847	N	MET	A	115	27.161	43.744	78.347	1.00	12.86	A
	ATOM 5848	CA	MET	A	115	27.986	44.876	78.750	1.00	11.47	A
15	ATOM 5849	CB	MET	A	115	29.219	44.375	79.516	1.00	14.17	A
	ATOM 5850	CG	MET	A	115	30.295	45.433	79.785	1.00	19.50	A
	ATOM 5851	SD	MET	A	115	31.315	45.040	81.253	1.00	26.29	A
	ATOM 5852	CE	MET	A	115	31.200	46.546	82.323	1.00	25.88	A
	ATOM 5853	C	MET	A	115	28.398	45.721	77.546	1.00	10.85	A
20	ATOM 5854	O	MET	A	115	28.364	46.951	77.602	1.00	10.44	A
	ATOM 5855	N	PHE	A	116	28.786	45.063	76.458	1.00	10.25	A
	ATOM 5856	CA	PHE	A	116	29.172	45.783	75.249	1.00	9.42	A
	ATOM 5857	CB	PHE	A	116	29.552	44.810	74.126	1.00	9.27	A
	ATOM 5858	CG	PHE	A	116	31.026	44.519	74.038	1.00	11.09	A
25	ATOM 5859	CD1	PHE	A	116	31.687	43.865	75.070	1.00	10.32	A

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	ATOM 5860	CD2	PHE	A	116	31.749	44.897	72.912	1.00	12.11	A
	ATOM 5861	CE1	PHE	A	116	33.053	43.589	74.985	1.00	12.71	A
	ATOM 5862	CE2	PHE	A	116	33.113	44.629	72.814	1.00	11.83	A
	ATOM 5863	CZ	PHE	A	116	33.766	43.972	73.853	1.00	11.75	A
5	ATOM 5864	C	PHE	A	116	28.013	46.652	74.772	1.00	7.94	A
	ATOM 5865	O	PHE	A	116	28.193	47.826	74.460	1.00	8.19	A
	ATOM 6152	N	TYR	A	152	44.548	57.094	66.166	1.00	5.28	A
	ATOM 6153	CA	TYR	A	152	43.884	56.348	67.225	1.00	4.93	A
	ATOM 6154	CB	TYR	A	152	44.409	56.744	68.612	1.00	5.14	A
10	ATOM 6155	CG	TYR	A	152	44.300	55.605	69.611	1.00	5.38	A
	ATOM 6156	CD1	TYR	A	152	44.726	54.319	69.273	1.00	6.68	A
	ATOM 6157	CE1	TYR	A	152	44.646	53.268	70.177	1.00	6.58	A
	ATOM 6158	CD2	TYR	A	152	43.784	55.806	70.888	1.00	4.95	A
	ATOM 6159	CE2	TYR	A	152	43.702	54.755	71.804	1.00	4.84	A
15	ATOM 6160	CZ	TYR	A	152	44.136	53.492	71.439	1.00	5.18	A
	ATOM 6161	OH	TYR	A	152	44.081	52.443	72.330	1.00	6.87	A
	ATOM 6162	C	TYR	A	152	42.372	56.492	67.156	1.00	5.08	A
	ATOM 6163	O	TYR	A	152	41.647	55.557	67.485	1.00	5.51	A
	ATOM 6164	N	TRP	A	153	41.884	57.656	66.736	1.00	5.39	A
20	ATOM 6165	CA	TRP	A	153	40.442	57.818	66.600	1.00	5.76	A
	ATOM 6166	CB	TRP	A	153	40.073	59.242	66.171	1.00	5.97	A
	ATOM 6167	CG	TRP	A	153	38.665	59.325	65.648	1.00	5.87	A
	ATOM 6168	CD2	TRP	A	153	37.471	58.920	66.332	1.00	5.91	A
	ATOM 6169	CE2	TRP	A	153	36.396	59.086	65.429	1.00	5.96	A
25	ATOM 6170	CE3	TRP	A	153	37.207	58.420	67.615	1.00	6.22	A

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	ATOM 6171	CD1	TRP	A	153	38.274	59.723	64.399	1.00	7.17	A
	ATOM 6172	NE1	TRP	A	153	36.912	59.582	64.261	1.00	7.77	A
	ATOM 6173	CZ2	TRP	A	153	35.072	58.781	65.772	1.00	6.91	A
	ATOM 6174	CZ3	TRP	A	153	35.886	58.116	67.956	1.00	7.15	A
5	ATOM 6175	CH2	TRP	A	153	34.839	58.294	67.032	1.00	7.76	A
	ATOM 6176	C	TRP	A	153	39.930	56.835	65.546	1.00	5.37	A
	ATOM 6177	O	TRP	A	153	38.934	56.144	65.756	1.00	5.17	A
	ATOM 6178	N	GLU	A	154	40.611	56.772	64.406	1.00	5.96	A
	ATOM 6179	CA	GLU	A	154	40.176	55.877	63.343	1.00	5.72	A
10	ATOM 6180	CB	GLU	A	154	41.009	56.110	62.079	1.00	6.13	A
	ATOM 6181	CG	GLU	A	154	40.449	55.429	60.833	1.00	6.44	A
	ATOM 6182	CD	GLU	A	154	40.878	53.979	60.703	1.00	6.70	A
	ATOM 6183	OE1	GLU	A	154	40.229	53.235	59.938	1.00	8.97	A
	ATOM 6184	OE2	GLU	A	154	41.876	53.586	61.345	1.00	8.06	A
15	ATOM 6185	C	GLU	A	154	40.247	54.414	63.774	1.00	5.12	A
	ATOM 6186	O	GLU	A	154	39.355	53.625	63.467	1.00	6.20	A
	ATOM 6187	N	ILE	A	155	41.305	54.059	64.497	1.00	5.18	A
	ATOM 6188	CA	ILE	A	155	41.489	52.696	64.975	1.00	4.86	A
	ATOM 6189	CB	ILE	A	155	42.901	52.549	65.580	1.00	5.47	A
20	ATOM 6190	CG2	ILE	A	155	42.987	51.319	66.475	1.00	6.67	A
	ATOM 6191	CG1	ILE	A	155	43.925	52.501	64.440	1.00	5.20	A
	ATOM 6192	CD1	ILE	A	155	45.357	52.705	64.879	1.00	6.49	A
	ATOM 6193	C	ILE	A	155	40.413	52.296	65.987	1.00	5.58	A
	ATOM 6194	O	ILE	A	155	39.780	51.247	65.851	1.00	5.20	A
25	ATOM 6195	N	CYS	A	156	40.196	53.136	66.992	1.00	4.65	A

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	ATOM 6196	CA	CYS A 156	39.190	52.838	68.007	1.00	5.13	A
	ATOM 6197	CB	CYS A 156	39.216	53.888	69.121	1.00	5.71	A
	ATOM 6198	SG	CYS A 156	40.667	53.829	70.192	1.00	6.49	A
	ATOM 6199	C	CYS A 156	37.789	52.779	67.420	1.00	5.66	A
5	ATOM 6200	O	CYS A 156	37.026	51.855	67.710	1.00	6.21	A
	ATOM 6201	N	SER A 157	37.448	53.766	66.594	1.00	6.00	A
	ATOM 6202	CA	SER A 157	36.114	53.797	66.009	1.00	5.99	A
	ATOM 6203	CB	SER A 157	35.843	55.146	65.317	1.00	6.89	A
	ATOM 6204	OG	SER A 157	36.766	55.420	64.282	1.00	6.66	A
10	ATOM 6205	C	SER A 157	35.868	52.633	65.053	1.00	6.25	A
	ATOM 6206	O	SER A 157	34.746	52.146	64.952	1.00	6.68	A
	ATOM 6207	N	THR A 158	36.902	52.170	64.358	1.00	6.04	A
	ATOM 6208	CA	THR A 158	36.717	51.043	63.452	1.00	6.77	A
	ATOM 6209	CB	THR A 158	38.027	50.693	62.720	1.00	7.66	A
15	ATOM 6210	OG1	THR A 158	38.194	51.589	61.617	1.00	8.90	A
	ATOM 6211	CG2	THR A 158	38.004	49.253	62.214	1.00	8.99	A
	ATOM 6212	C	THR A 158	36.219	49.827	64.225	1.00	7.46	A
	ATOM 6213	O	THR A 158	35.299	49.137	63.792	1.00	7.44	A
	ATOM 6214	N	THR A 159	36.813	49.572	65.380	1.00	6.82	A
20	ATOM 6215	CA	THR A 159	36.400	48.428	66.174	1.00	8.47	A
	ATOM 6216	CB	THR A 159	37.480	48.070	67.201	1.00	8.32	A
	ATOM 6217	OG1	THR A 159	38.641	47.615	66.494	1.00	9.56	A
	ATOM 6218	CG2	THR A 159	37.005	46.971	68.140	1.00	8.90	A
	ATOM 6219	C	THR A 159	35.049	48.651	66.849	1.00	7.49	A
25	ATOM 6220	O	THR A 159	34.222	47.740	66.900	1.00	8.33	A

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	ATOM 6221	N	LEU A 160	34.804	49.857	67.354	1.00	6.78	A
	ATOM 6222	CA	LEU A 160	33.519	50.125	67.988	1.00	6.38	A
	ATOM 6223	CB	LEU A 160	33.498	51.531	68.588	1.00	6.84	A
	ATOM 6224	CG	LEU A 160	34.480	51.773	69.736	1.00	8.63	A
5	ATOM 6225	CD1	LEU A 160	34.360	53.209	70.217	1.00	11.20	A
	ATOM 6226	CD2	LEU A 160	34.194	50.799	70.871	1.00	11.27	A
	ATOM 6227	C	LEU A 160	32.384	49.979	66.974	1.00	7.24	A
	ATOM 6228	O	LEU A 160	31.300	49.503	67.311	1.00	7.48	A
	ATOM 6229	N	LEU A 161	32.642	50.383	65.733	1.00	6.66	A
10	ATOM 6230	CA	LEU A 161	31.641	50.297	64.673	1.00	8.42	A
	ATOM 6231	CB	LEU A 161	32.156	50.972	63.403	1.00	9.08	A
	ATOM 6232	CG	LEU A 161	32.054	52.499	63.404	1.00	8.17	A
	ATOM 6233	CD1	LEU A 161	32.903	53.074	62.283	1.00	9.90	A
	ATOM 6234	CD2	LEU A 161	30.594	52.915	63.251	1.00	9.54	A
15	ATOM 6235	C	LEU A 161	31.232	48.862	64.366	1.00	8.60	A
	ATOM 6236	O	LEU A 161	30.132	48.619	63.874	1.00	9.07	A
	ATOM 6237	N	VAL A 162	32.116	47.914	64.652	1.00	8.54	A
	ATOM 6238	CA	VAL A 162	31.806	46.511	64.421	1.00	10.19	A
	ATOM 6239	CB	VAL A 162	33.025	45.605	64.724	1.00	9.33	A
20	ATOM 6240	CG1	VAL A 162	32.617	44.139	64.661	1.00	12.54	A
	ATOM 6241	CG2	VAL A 162	34.147	45.883	63.735	1.00	10.70	A
	ATOM 6242	C	VAL A 162	30.656	46.102	65.337	1.00	10.61	A
	ATOM 6243	O	VAL A 162	29.756	45.367	64.933	1.00	12.29	A
	ATOM 6244	N	PHE A 163	30.685	46.593	66.574	1.00	9.62	A
25	ATOM 6245	CA	PHE A 163	29.657	46.250	67.550	1.00	9.97	A

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	ATOM 6246	CB	PHE A 163	30.284	46.124	68.940	1.00	10.40	A
	ATOM 6247	CG	PHE A 163	31.388	45.111	69.010	1.00	13.43	A
	ATOM 6248	CD1	PHE A 163	32.699	45.461	68.698	1.00	14.97	A
	ATOM 6249	CD2	PHE A 163	31.112	43.796	69.360	1.00	16.10	A
5	ATOM 6250	CE1	PHE A 163	33.718	44.511	68.735	1.00	16.79	A
	ATOM 6251	CE2	PHE A 163	32.118	42.846	69.398	1.00	17.88	A
	ATOM 6252	CZ	PHE A 163	33.428	43.199	69.086	1.00	18.31	A
	ATOM 6253	C	PHE A 163	28.476	47.214	67.605	1.00	9.96	A
	ATOM 6254	O	PHE A 163	27.414	46.865	68.116	1.00	10.98	A
10	ATOM 6528	N	THR A 197	41.100	40.642	60.451	1.00	6.55	A
	ATOM 6529	CA	THR A 197	40.708	40.042	61.711	1.00	6.54	A
	ATOM 6530	CB	THR A 197	41.867	40.118	62.727	1.00	7.01	A
	ATOM 6531	OG1	THR A 197	42.283	41.481	62.890	1.00	6.91	A
	ATOM 6532	CG2	THR A 197	43.048	39.300	62.229	1.00	7.77	A
15	ATOM 6533	C	THR A 197	39.489	40.776	62.251	1.00	6.16	A
	ATOM 6534	O	THR A 197	39.252	41.929	61.910	1.00	7.50	A
	ATOM 6535	N	LYS A 198	38.708	40.110	63.091	1.00	7.12	A
	ATOM 6536	CA	LYS A 198	37.522	40.742	63.647	1.00	7.25	A
	ATOM 6537	CB	LYS A 198	36.729	39.729	64.481	1.00	9.37	A
20	ATOM 6538	CG	LYS A 198	35.536	40.316	65.222	1.00	12.51	A
	ATOM 6539	CD	LYS A 198	34.529	40.978	64.294	1.00	16.24	A
	ATOM 6540	CE	LYS A 198	33.878	39.974	63.358	1.00	16.57	A
	ATOM 6541	NZ	LYS A 198	32.726	40.573	62.615	1.00	16.81	A
	ATOM 6542	C	LYS A 198	37.910	41.945	64.507	1.00	7.23	A
25	ATOM 6543	O	LYS A 198	37.377	43.043	64.331	1.00	8.34	A

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	ATOM 6544	N	LEU A 199	38.853	41.729	65.419	1.00	7.65	A
	ATOM 6545	CA	LEU A 199	39.316	42.775	66.325	1.00	7.68	A
	ATOM 6546	CB	LEU A 199	39.247	42.283	67.772	1.00	10.39	A
	ATOM 6547	CG	LEU A 199	37.902	41.731	68.242	1.00	12.70	A
5	ATOM 6548	CD1	LEU A 199	38.057	41.197	69.652	1.00	15.45	A
	ATOM 6549	CD2	LEU A 199	36.837	42.817	68.182	1.00	14.13	A
	ATOM 6550	C	LEU A 199	40.735	43.235	66.028	1.00	7.07	A
	ATOM 6551	OT1	LEU A 199	41.384	42.659	65.131	1.00	7.11	A
	ATOM 6552	OT2	LEU A 199	41.186	44.168	66.721	1.00	8.05	A
10	ATOM 6613	N1	GSH H 200	47.240	49.426	78.365	1.00	5.76	H
	ATOM 6614	CA1	GSH H 200	48.071	48.329	77.882	1.00	6.49	H
	ATOM 6615	C1	GSH H 200	48.552	48.593	76.433	1.00	5.96	H
	ATOM 6616	O11	GSH H 200	47.961	49.446	75.764	1.00	6.16	H
	ATOM 6617	O12	GSH H 200	49.623	47.939	76.023	1.00	5.89	H
15	ATOM 6618	CB1	GSH H 200	47.193	47.058	77.940	1.00	7.07	H
	ATOM 6619	CG1	GSH H 200	47.971	45.743	77.668	1.00	7.43	H
	ATOM 6620	CD1	GSH H 200	46.947	44.584	77.671	1.00	7.37	H
	ATOM 6621	OE1	GSH H 200	46.223	44.381	78.652	1.00	7.91	H
	ATOM 6622	N2	GSH H 200	47.074	43.729	76.649	1.00	6.87	H
20	ATOM 6623	CA2	GSH H 200	46.310	42.477	76.623	1.00	6.95	H
	ATOM 6624	C2	GSH H 200	47.130	41.349	77.273	1.00	8.08	H
	ATOM 6625	O2	GSH H 200	48.345	41.290	77.178	1.00	8.04	H
	ATOM 6626	CB2	GSH H 200	46.025	42.056	75.164	1.00	7.00	H
	ATOM 6627	SG2	GSH H 200	44.867	43.164	74.287	1.00	8.63	H
25	ATOM 6628	N3	GSH H 200	46.473	40.585	78.154	1.00	10.11	H

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	ATOM 6629	CA3	GSH	H	200	47.063	39.404	78.824	1.00	12.26	H
	ATOM 6630	C3	GSH	H	200	46.455	39.280	80.221	1.00	14.36	H
	ATOM 6631	O31	GSH	H	200	46.823	38.312	80.902	1.00	17.27	H
	ATOM 6632	O32	GSH	H	200	45.621	40.144	80.600	1.00	17.25	H
5	ATOM 6677	OH2	WAT	S	1	45.932	55.216	78.140	1.00	11.00	S
	ATOM 6678	OH2	WAT	S	2	44.001	53.704	79.474	1.00	8.61	S
	ATOM 6679	OH2	WAT	S	3	45.044	54.147	82.027	1.00	9.47	S
	ATOM 6680	OH2	WAT	S	4	47.066	56.184	80.641	1.00	11.51	S
	ATOM 6681	OH2	WAT	S	5	44.400	56.542	80.238	1.00	6.66	S
10	ATOM 6682	OH2	WAT	S	6	46.942	53.261	80.035	1.00	7.38	S
	ATOM 6689	OH2	WAT	S	13	44.802	42.314	61.828	1.00	6.00	S
	ATOM 6692	OH2	WAT	S	16	46.602	44.435	61.593	1.00	6.08	S
	ATOM 6693	OH2	WAT	S	17	51.844	46.380	76.801	1.00	5.53	S
	ATOM 6694	OH2	WAT	S	18	46.016	50.205	68.769	1.00	4.93	S
15	ATOM 6697	OH2	WAT	S	21	46.289	50.659	71.607	1.00	6.24	S
	ATOM 6699	OH2	WAT	S	23	51.226	46.303	81.832	1.00	7.26	S
	ATOM 6701	OH2	WAT	S	25	49.891	52.595	76.855	1.00	6.35	S
	ATOM 6702	OH2	WAT	S	26	52.165	42.023	65.879	1.00	6.86	S
	ATOM 6703	OH2	WAT	S	27	54.167	43.535	79.506	1.00	6.85	S
20	ATOM 6714	OH2	WAT	S	38	47.233	52.192	77.524	1.00	8.27	S
	ATOM 6718	OH2	WAT	S	42	48.563	46.768	84.725	1.00	8.57	S
	ATOM 6719	OH2	WAT	S	43	58.660	41.683	70.327	1.00	7.93	S
	ATOM 6733	OH2	WAT	S	57	48.526	46.955	81.917	1.00	7.89	S
	ATOM 6748	OH2	WAT	S	72	39.916	39.195	66.189	1.00	12.20	S
25	ATOM 6762	OH2	WAT	S	88	52.225	56.098	78.210	1.00	11.05	S

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	ATOM 6783	OH2 WAT S 109	41.879	49.920	62.315	1.00	9.83	S
	ATOM 6784	OH2 WAT S 110	41.843	43.595	60.246	1.00	7.19	S
	ATOM 6788	OH2 WAT S 114	50.291	44.524	83.978	1.00	11.55	S
	ATOM 6791	OH2 WAT S 117	45.204	49.983	75.259	1.00	11.59	S
5	ATOM 6794	OH2 WAT S 121	36.093	43.586	61.844	1.00	10.06	S
	ATOM 6812	OH2 WAT S 140	46.502	35.525	67.908	1.00	16.03	S
	ATOM 6818	OH2 WAT S 146	46.548	45.276	81.207	1.00	11.87	S
	ATOM 6848	OH2 WAT S 177	47.305	35.643	80.850	1.00	15.13	S
	ATOM 6851	OH2 WAT S 180	42.393	49.873	82.928	1.00	14.77	S
10	ATOM 6888	OH2 WAT S 219	49.260	57.057	77.605	1.00	11.44	S
	ATOM 6894	OH2 WAT S 225	39.600	37.346	63.532	1.00	14.35	S
	ATOM 6908	OH2 WAT S 239	44.676	42.614	80.064	1.00	17.81	S
	ATOM 6923	OH2 WAT S 256	51.755	42.823	85.972	1.00	15.23	S
	ATOM 6936	OH2 WAT S 269	43.744	50.995	80.612	1.00	22.66	S
15	ATOM 6977	OH2 WAT S 310	41.854	37.441	65.183	1.00	14.71	S
	ATOM 6988	OH2 WAT S 321	52.715	31.754	68.251	1.00	25.02	S
	ATOM 7004	OH2 WAT S 338	47.955	36.940	60.191	1.00	23.06	S
	ATOM 7020	OH2 WAT S 356	52.697	38.727	84.915	1.00	25.89	S
	ATOM 7035	OH2 WAT S 371	52.695	46.000	79.504	1.00	6.20	S
20	ATOM 7044	OH2 WAT S 380	45.939	45.946	85.168	1.00	15.59	S
	ATOM 7069	OH2 WAT S 409	58.139	37.692	70.855	1.00	19.42	S
	ATOM 7121	OH2 WAT S 463	44.454	49.864	78.620	1.00	17.85	S
	ATOM 7141	OH2 WAT S 486	38.783	46.154	59.815	1.00	18.01	S
	ATOM 7185	OH2 WAT S 533	55.398	32.865	68.634	1.00	26.34	S
25	ATOM 7218	OH2 WAT S 568	39.362	52.746	81.658	1.00	20.82	S

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	ATOM 7276	OH2 WAT S	630	54.033	36.951	83.283	1.00	30.87	S
	ATOM 7291	OH2 WAT S	647	59.120	37.414	73.286	1.00	30.13	S
	ATOM 7297	OH2 WAT S	653	43.339	48.112	81.026	1.00	26.20	S
	ATOM 7315	OH2 WAT S	677	41.879	54.425	82.374	1.00	22.86	S
5	ATOM 7345	OH2 WAT S	707	49.594	41.237	85.951	1.00	26.42	S
	ATOM 7396	OH2 WAT S	760	33.326	48.774	82.446	1.00	41.01	S
	ATOM 7397	OH2 WAT S	761	44.428	46.156	82.727	1.00	21.46	S
	ATOM 7432	OH2 WAT S	798	37.760	35.933	64.870	1.00	24.86	S
	ATOM 7447	OH2 WAT S	815	44.586	33.922	63.810	1.00	27.17	S
10	ATOM 7451	OH2 WAT S	819	42.590	49.990	76.103	1.00	37.29	S
	ATOM 7491	OH2 WAT S	865	49.313	34.257	64.053	1.00	23.25	S
	ATOM 7551	OH2 WAT S	936	38.403	45.727	86.224	1.00	34.77	S
	ATOM 7559	OH2 WAT S	947	39.267	36.269	81.440	1.00	35.93	S
	ATOM 7562	OH2 WAT S	950	46.311	34.424	83.694	1.00	37.47	S
15	ATOM 7566	OH2 WAT S	954	49.354	35.076	61.559	1.00	34.30	S
	ATOM 7573	OH2 WAT S	962	41.074	48.947	64.727	1.00	6.62	S
	ATOM 7576	OH2 WAT S	965	42.360	48.144	66.991	1.00	8.16	S
	ATOM 7580	OH2 WAT S	969	40.070	46.736	70.359	1.00	15.63	S
	ATOM 7581	OH2 WAT S	970	40.472	46.466	67.816	1.00	11.14	S
20	ATOM 7584	OH2 WAT S	974	46.488	28.447	69.078	1.00	22.47	S
	ATOM 7664	OH2 WAT S	1104	49.140	39.068	82.273	1.00	19.35	S
	ATOM 7673	OH2 WAT S	1117	49.385	36.341	85.538	1.00	28.59	S
	ATOM 7675	OH2 WAT S	1119	41.071	46.806	79.458	1.00	26.70	S
	ATOM 7676	OH2 WAT S	1120	38.224	37.620	67.988	1.00	32.98	S
25	ATOM 7678	OH2 WAT S	1123	41.996	35.058	66.930	1.00	32.93	S

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	ATOM 7683	OH2	WAT	S1129	47.152	42.956	85.367	1.00	37.94	S
	ATOM 7722	OH2	WAT	S1180	36.068	36.649	75.341	1.00	43.94	S
	ATOM 7732	OH2	WAT	S1191	42.482	52.407	81.689	1.00	21.38	S
	ATOM 7733	OH2	WAT	S1192	39.535	50.355	82.874	1.00	32.24	S
5	ATOM 7737	OH2	WAT	S1196	50.213	38.953	84.774	1.00	27.44	S
	ATOM 7843	OH2	WAT	S1339	35.818	45.711	82.635	1.00	44.01	S
	ATOM 7853	OH2	WAT	S1354	46.962	39.117	87.092	1.00	36.93	S
	ATOM 7874	OH2	WAT	S1383	32.545	41.137	82.654	1.00	33.68	S
	ATOM 7884	OH2	WAT	S1401	45.736	37.693	83.360	1.00	44.69	S
10	ATOM 7926	OH2	WAT	S1447	45.667	30.953	67.849	1.00	35.68	S
	ATOM 7927	OH2	WAT	S1448	55.702	38.128	82.442	1.00	36.01	S
	ATOM 7948	OH2	WAT	S1474	44.404	43.677	86.488	1.00	42.40	S
	ATOM 7952	OH2	WAT	S1480	40.448	40.603	87.707	1.00	38.53	S
	ATOM 7954	OH2	WAT	S1482	48.226	42.042	87.524	1.00	41.24	S
15	ATOM 7996	OH2	WAT	S1530	41.155	35.723	62.708	1.00	35.51	S
	ATOM 8019	OH2	WAT	S1558	44.128	34.781	68.900	1.00	42.94	S
	ATOM 8020	OH2	WAT	S1559	43.571	35.946	71.823	1.00	42.74	S
	ATOM 8127	C1	U46	X 201	41.871	38.419	75.254	1.00	41.44	X
	ATOM 8128	C2	U46	X 201	40.838	38.243	74.213	1.00	41.53	X
20	ATOM 8129	C3	U46	X 201	40.546	39.776	73.818	1.00	41.45	X
	ATOM 8130	C4	U46	X 201	42.010	40.338	73.856	1.00	41.07	X
	ATOM 8131	C5	U46	X 201	42.792	39.065	74.274	1.00	41.56	X
	ATOM 8132	O6	U46	X 201	42.922	38.036	73.307	1.00	41.32	X
	ATOM 8133	C7	U46	X 201	41.676	37.405	73.215	1.00	41.76	X
25	ATOM 8134	C14	U46	X 201	42.399	41.346	74.949	1.00	40.61	X

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	ATOM 8135	C16	U46	X	201	41.701	42.023	75.922	1.00	40.28	X
	ATOM 8136	C18	U46	X	201	42.762	42.478	76.971	1.00	40.54	X
	ATOM 8137	C20	U46	X	201	42.973	41.118	77.340	1.00	40.10	X
	ATOM 8138	C21	U46	X	201	43.792	40.318	78.232	1.00	39.99	X
5	ATOM 8139	C24	U46	X	201	43.404	38.935	77.644	1.00	40.60	X
	ATOM 8140	C27	U46	X	201	43.941	37.551	78.094	1.00	41.02	X
	ATOM 8141	C30	U46	X	201	43.168	36.476	77.301	1.00	41.85	X
	ATOM 8142	O36	U46	X	201	42.312	43.249	77.943	1.00	40.95	X
	ATOM 8143	C39	U46	X	201	39.913	39.986	72.481	1.00	41.80	X
10	ATOM 8144	C41	U46	X	201	38.932	38.921	72.298	1.00	42.50	X
	ATOM 8145	C44	U46	X	201	37.645	38.825	72.466	1.00	43.42	X
	ATOM 8146	C46	U46	X	201	36.596	39.762	72.916	1.00	43.47	X
	ATOM 8147	C48	U46	X	201	35.496	39.760	71.872	1.00	44.38	X
	ATOM 8148	C51	U46	X	201	34.385	40.531	72.463	1.00	45.27	X
15	ATOM 8149	C54	U46	X	201	33.109	40.654	71.681	1.00	45.90	X
	ATOM 8150	O57	U46	X	201	32.181	41.256	72.479	1.00	46.00	X
	ATOM 8151	O58	U46	X	201	32.887	40.235	70.603	1.00	46.55	X

Table 5

20 Three-dimensional structural coordinate of the complex of human hematopoietic PGDS with calcium, glutathione and 9,11-dideoxy -9 α ,11 α -epoxymethanoprostaglandine F_{2 α} (U44)

	ATOM 4966	N	TYR	A	8	24.336	32.545	34.593	1.00	23.71	A
25	ATOM 4967	CA	TYR	A	8	22.908	32.784	34.729	1.00	23.39	A

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	ATOM 4968	CB	TYR	A	8	22.170	31.441	34.781	1.00	22.82	A
	ATOM 4969	CG	TYR	A	8	20.663	31.544	34.721	1.00	22.10	A
	ATOM 4970	CD1	TYR	A	8	20.024	32.094	33.606	1.00	21.74	A
	ATOM 4971	CE1	TYR	A	8	18.634	32.184	33.541	1.00	21.38	A
5	ATOM 4972	CD2	TYR	A	8	19.872	31.084	35.777	1.00	21.64	A
	ATOM 4973	CE2	TYR	A	8	18.481	31.170	35.723	1.00	21.52	A
	ATOM 4974	CZ	TYR	A	8	17.872	31.721	34.602	1.00	21.33	A
	ATOM 4975	OH	TYR	A	8	16.504	31.801	34.542	1.00	21.12	A
	ATOM 4976	C	TYR	A	8	22.659	33.572	36.016	1.00	23.34	A
10	ATOM 4977	O	TYR	A	8	23.597	33.866	36.755	1.00	23.65	A
	ATOM 4978	N	PHE	A	9	21.402	33.921	36.273	1.00	23.18	A
	ATOM 4979	CA	PHE	A	9	21.042	34.657	37.478	1.00	23.08	A
	ATOM 4980	CB	PHE	A	9	19.635	35.237	37.348	1.00	23.27	A
	ATOM 4981	CG	PHE	A	9	19.527	36.344	36.342	1.00	23.76	A
15	ATOM 4982	CD1	PHE	A	9	18.642	36.248	35.273	1.00	23.77	A
	ATOM 4983	CD2	PHE	A	9	20.298	37.494	36.471	1.00	24.01	A
	ATOM 4984	CE1	PHE	A	9	18.524	37.286	34.346	1.00	24.05	A
	ATOM 4985	CE2	PHE	A	9	20.190	38.535	35.552	1.00	24.19	A
	ATOM 4986	CZ	PHE	A	9	19.300	38.431	34.488	1.00	24.13	A
20	ATOM 4987	C	PHE	A	9	21.085	33.712	38.666	1.00	22.94	A
	ATOM 4988	O	PHE	A	9	21.182	32.497	38.491	1.00	22.79	A
	ATOM 4989	N	ASN	A	10	21.014	34.263	39.873	1.00	22.88	A
	ATOM 4990	CA	ASN	A	10	21.039	33.427	41.064	1.00	22.79	A
	ATOM 4991	CB	ASN	A	10	21.504	34.217	42.288	1.00	22.91	A
25	ATOM 4992	CG	ASN	A	10	21.505	33.369	43.546	1.00	22.98	A

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	ATOM 4993	OD1 ASN A	10	21.877	32.191	43.508	1.00	22.82	A
	ATOM 4994	ND2 ASN A	10	21.091	33.957	44.666	1.00	23.07	A
	ATOM 4995	C ASN A	10	19.674	32.817	41.345	1.00	22.64	A
	ATOM 4996	O ASN A	10	18.942	33.272	42.225	1.00	22.44	A
5	ATOM 4997	N MET A	11	19.340	31.785	40.576	1.00	22.50	A
	ATOM 4998	CA MET A	11	18.080	31.070	40.723	1.00	22.24	A
	ATOM 4999	CB MET A	11	16.895	31.982	40.360	1.00	23.52	A
	ATOM 5000	CG MET A	11	17.007	32.727	39.047	1.00	24.37	A
	ATOM 5001	SD MET A	11	15.802	34.129	38.850	1.00	26.46	A
10	ATOM 5002	CE MET A	11	16.836	35.517	39.396	1.00	25.81	A
	ATOM 5003	C MET A	11	18.090	29.814	39.857	1.00	21.50	A
	ATOM 5004	O MET A	11	18.967	29.645	39.006	1.00	21.28	A
	ATOM 5005	N ARG A	12	17.141	28.916	40.107	1.00	20.53	A
	ATOM 5006	CA ARG A	12	17.043	27.684	39.339	1.00	19.59	A
15	ATOM 5007	CB ARG A	12	15.934	26.791	39.911	1.00	19.37	A
	ATOM 5008	CG ARG A	12	16.161	26.371	41.367	1.00	19.34	A
	ATOM 5009	CD ARG A	12	15.131	25.327	41.823	1.00	18.54	A
	ATOM 5010	NE ARG A	12	13.767	25.844	41.732	1.00	18.63	A
	ATOM 5011	CZ ARG A	12	13.276	26.789	42.524	1.00	18.61	A
20	ATOM 5012	NH1 ARG A	12	14.038	27.316	43.477	1.00	18.60	A
	ATOM 5013	NH2 ARG A	12	12.033	27.219	42.354	1.00	18.16	A
	ATOM 5014	C ARG A	12	16.720	28.094	37.909	1.00	19.15	A
	ATOM 5015	O ARG A	12	17.536	27.922	37.003	1.00	18.76	A
	ATOM 5016	N GLY A	13	15.531	28.659	37.729	1.00	18.65	A
25	ATOM 5017	CA GLY A	13	15.102	29.119	36.421	1.00	18.28	A

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	ATOM 5018	C	GLY A	13	15.414	28.194	35.262	1.00	18.14	A
	ATOM 5019	O	GLY A	13	15.277	26.972	35.366	1.00	17.63	A
	ATOM 5020	N	ARG A	14	15.863	28.793	34.162	1.00	17.96	A
	ATOM 5021	CA	ARG A	14	16.177	28.069	32.933	1.00	18.29	A
5	ATOM 5022	CB	ARG A	14	16.047	29.022	31.738	1.00	18.89	A
	ATOM 5023	CG	ARG A	14	14.666	29.644	31.606	1.00	19.92	A
	ATOM 5024	CD	ARG A	14	14.549	30.514	30.365	1.00	21.37	A
	ATOM 5025	NE	ARG A	14	13.164	30.648	29.917	1.00	22.61	A
	ATOM 5026	CZ	ARG A	14	12.361	31.673	30.191	1.00	23.60	A
10	ATOM 5027	NH1	ARG A	14	11.110	31.677	29.727	1.00	24.26	A
	ATOM 5028	NH2	ARG A	14	12.799	32.701	30.906	1.00	23.64	A
	ATOM 5029	C	ARG A	14	17.552	27.412	32.912	1.00	18.18	A
	ATOM 5030	O	ARG A	14	17.885	26.703	31.970	1.00	18.06	A
	ATOM 5031	N	ALA A	15	18.355	27.634	33.943	1.00	18.06	A
15	ATOM 5032	CA	ALA A	15	19.680	27.027	33.964	1.00	18.18	A
	ATOM 5033	CB	ALA A	15	20.689	27.991	34.579	1.00	18.24	A
	ATOM 5034	C	ALA A	15	19.694	25.710	34.735	1.00	18.01	A
	ATOM 5035	O	ALA A	15	20.576	24.875	34.541	1.00	17.87	A
	ATOM 5036	N	GLU A	16	18.712	25.520	35.607	1.00	18.14	A
20	ATOM 5037	CA	GLU A	16	18.671	24.313	36.426	1.00	17.94	A
	ATOM 5038	CB	GLU A	16	17.412	24.314	37.295	1.00	18.23	A
	ATOM 5039	CG	GLU A	16	17.518	23.451	38.545	1.00	18.77	A
	ATOM 5040	CD	GLU A	16	18.639	23.897	39.478	1.00	19.23	A
	ATOM 5041	OE1	GLU A	16	19.109	25.046	39.354	1.00	19.68	A
25	ATOM 5042	OE2	GLU A	16	19.043	23.099	40.349	1.00	19.82	A

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	ATOM 5043	C	GLU	A	16	18.774	22.991	35.653	1.00	17.71	A
	ATOM 5044	O	GLU	A	16	19.443	22.063	36.102	1.00	17.63	A
	ATOM 5045	N	ILE	A	17	18.124	22.900	34.497	1.00	17.52	A
	ATOM 5046	CA	ILE	A	17	18.176	21.667	33.715	1.00	17.48	A
5	ATOM 5047	CB	ILE	A	17	17.312	21.776	32.436	1.00	17.22	A
	ATOM 5048	CG2	ILE	A	17	17.790	22.941	31.585	1.00	17.01	A
	ATOM 5049	CG1	ILE	A	17	17.366	20.462	31.652	1.00	17.08	A
	ATOM 5050	CD1	ILE	A	17	16.797	19.262	32.406	1.00	17.66	A
	ATOM 5051	C	ILE	A	17	19.611	21.316	33.330	1.00	17.59	A
10	ATOM 5052	O	ILE	A	17	19.977	20.143	33.255	1.00	17.72	A
	ATOM 5242	N	TRP	A	39	24.145	42.736	35.174	1.00	42.17	A
	ATOM 5243	CA	TRP	A	39	23.529	42.160	33.983	1.00	41.90	A
	ATOM 5244	CB	TRP	A	39	22.062	41.812	34.261	1.00	41.67	A
	ATOM 5245	CG	TRP	A	39	21.310	41.341	33.047	1.00	41.34	A
15	ATOM 5246	CD2	TRP	A	39	21.735	40.353	32.097	1.00	41.24	A
	ATOM 5247	CE2	TRP	A	39	20.708	40.233	31.133	1.00	41.24	A
	ATOM 5248	CE3	TRP	A	39	22.881	39.559	31.967	1.00	41.17	A
	ATOM 5249	CD1	TRP	A	39	20.082	41.765	32.632	1.00	41.33	A
	ATOM 5250	NE1	TRP	A	39	19.713	41.106	31.484	1.00	41.21	A
20	ATOM 5251	CZ2	TRP	A	39	20.794	39.348	30.051	1.00	41.18	A
	ATOM 5252	CZ3	TRP	A	39	22.967	38.678	30.891	1.00	41.18	A
	ATOM 5253	CH2	TRP	A	39	21.927	38.582	29.947	1.00	41.22	A
	ATOM 5254	C	TRP	A	39	23.610	43.095	32.774	1.00	41.82	A
	ATOM 5255	O	TRP	A	39	23.990	42.678	31.681	1.00	41.83	A
25	ATOM 5256	N	PRO	A	40	23.253	44.376	32.956	1.00	41.74	A

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	ATOM 5257	CD	PRO	A	40	22.790	45.032	34.194	1.00	41.72	A
	ATOM 5258	CA	PRO	A	40	23.299	45.335	31.850	1.00	41.61	A
	ATOM 5259	CB	PRO	A	40	23.085	46.672	32.553	1.00	41.71	A
	ATOM 5260	CG	PRO	A	40	22.158	46.304	33.670	1.00	41.78	A
5	ATOM 5261	C	PRO	A	40	24.598	45.298	31.047	1.00	41.46	A
	ATOM 5262	O	PRO	A	40	24.571	45.278	29.818	1.00	41.46	A
	ATOM 5263	N	GLU	A	41	25.731	45.284	31.742	1.00	41.23	A
	ATOM 5264	CA	GLU	A	41	27.030	45.262	31.079	1.00	41.03	A
	ATOM 5265	CB	GLU	A	41	28.147	45.542	32.088	1.00	41.50	A
10	ATOM 5266	CG	GLU	A	41	27.983	46.835	32.868	1.00	42.28	A
	ATOM 5267	CD	GLU	A	41	26.844	46.776	33.870	1.00	42.66	A
	ATOM 5268	OE1	GLU	A	41	26.899	45.926	34.783	1.00	42.97	A
	ATOM 5269	OE2	GLU	A	41	25.895	47.579	33.746	1.00	43.13	A
	ATOM 5270	C	GLU	A	41	27.301	43.929	30.391	1.00	40.57	A
15	ATOM 5271	O	GLU	A	41	27.795	43.889	29.265	1.00	40.56	A
	ATOM 5272	N	ILE	A	42	26.977	42.839	31.078	1.00	39.94	A
	ATOM 5273	CA	ILE	A	42	27.193	41.499	30.547	1.00	39.34	A
	ATOM 5274	CB	ILE	A	42	26.899	40.434	31.624	1.00	39.29	A
	ATOM 5275	CG2	ILE	A	42	27.163	39.043	31.071	1.00	39.27	A
20	ATOM 5276	CG1	ILE	A	42	27.776	40.691	32.851	1.00	39.26	A
	ATOM 5277	CD1	ILE	A	42	27.446	39.819	34.036	1.00	39.48	A
	ATOM 5278	C	ILE	A	42	26.316	41.223	29.332	1.00	38.87	A
	ATOM 5279	O	ILE	A	42	26.780	40.678	28.331	1.00	38.77	A
	ATOM 5280	N	LYS	A	43	25.047	41.605	29.434	1.00	38.49	A
25	ATOM 5281	CA	LYS	A	43	24.077	41.404	28.363	1.00	38.12	A

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	ATOM 5282	CB	LYS	A	43	22.759	42.086	28.722	1.00	38.17	A
	ATOM 5283	CG	LYS	A	43	21.711	41.995	27.630	1.00	38.16	A
	ATOM 5284	CD	LYS	A	43	20.457	42.760	28.004	1.00	38.30	A
	ATOM 5285	CE	LYS	A	43	19.412	42.658	26.909	1.00	38.35	A
5	ATOM 5286	NZ	LYS	A	43	18.211	43.462	27.231	1.00	38.78	A
	ATOM 5287	C	LYS	A	43	24.555	41.940	27.021	1.00	37.94	A
	ATOM 5288	O	LYS	A	43	24.300	41.345	25.973	1.00	37.89	A
	ATOM 5328	N	GLY	A	49	22.030	38.588	23.868	1.00	27.57	A
	ATOM 5329	CA	GLY	A	49	21.714	39.214	25.141	1.00	26.68	A
10	ATOM 5330	C	GLY	A	49	20.783	38.447	26.055	1.00	26.11	A
	ATOM 5331	O	GLY	A	49	19.969	39.047	26.759	1.00	26.15	A
	ATOM 5332	N	LYS	A	50	20.902	37.124	26.055	1.00	25.32	A
	ATOM 5333	CA	LYS	A	50	20.058	36.286	26.899	1.00	24.83	A
	ATOM 5334	CB	LYS	A	50	18.987	35.584	26.055	1.00	25.06	A
15	ATOM 5335	CG	LYS	A	50	18.013	36.530	25.374	1.00	25.51	A
	ATOM 5336	CD	LYS	A	50	17.150	37.251	26.398	1.00	25.84	A
	ATOM 5337	CE	LYS	A	50	16.263	38.306	25.752	1.00	26.47	A
	ATOM 5338	NZ	LYS	A	50	15.382	37.745	24.694	1.00	26.77	A
	ATOM 5339	C	LYS	A	50	20.879	35.240	27.634	1.00	24.41	A
20	ATOM 5340	O	LYS	A	50	21.944	34.833	27.172	1.00	24.16	A
	ATOM 5341	N	ILE	A	51	20.383	34.825	28.794	1.00	23.98	A
	ATOM 5342	CA	ILE	A	51	21.045	33.800	29.586	1.00	23.81	A
	ATOM 5343	CB	ILE	A	51	21.654	34.373	30.889	1.00	23.59	A
	ATOM 5344	CG2	ILE	A	51	22.946	35.101	30.569	1.00	23.66	A
25	ATOM 5345	CG1	ILE	A	51	20.647	35.286	31.588	1.00	23.56	A

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	ATOM 5346	CD1	ILE	A	51	21.166	35.889	32.865	1.00	24.20	A
	ATOM 5347	C	ILE	A	51	20.012	32.737	29.925	1.00	23.69	A
	ATOM 5348	O	ILE	A	51	18.812	32.984	29.833	1.00	23.80	A
	ATOM 5349	N	PRO	A	52	20.461	31.545	30.341	1.00	23.80	A
5	ATOM 5350	CD	PRO	A	52	19.562	30.408	30.617	1.00	23.80	A
	ATOM 5351	CA	PRO	A	52	21.862	31.148	30.517	1.00	23.83	A
	ATOM 5352	CB	PRO	A	52	21.744	29.860	31.315	1.00	23.75	A
	ATOM 5353	CG	PRO	A	52	20.522	29.241	30.696	1.00	23.82	A
	ATOM 5354	C	PRO	A	52	22.657	30.935	29.234	1.00	24.05	A
10	ATOM 5355	O	PRO	A	52	22.107	30.869	28.132	1.00	23.56	A
	ATOM 5356	N	ILE	A	53	23.969	30.831	29.405	1.00	24.37	A
	ATOM 5357	CA	ILE	A	53	24.883	30.580	28.305	1.00	24.89	A
	ATOM 5358	CB	ILE	A	53	25.598	31.865	27.845	1.00	25.02	A
	ATOM 5359	CG2	ILE	A	53	24.582	32.851	27.265	1.00	25.04	A
15	ATOM 5360	CG1	ILE	A	53	26.353	32.488	29.018	1.00	25.09	A
	ATOM 5361	CD1	ILE	A	53	27.139	33.725	28.651	1.00	25.71	A
	ATOM 5362	C	ILE	A	53	25.920	29.600	28.830	1.00	25.23	A
	ATOM 5363	O	ILE	A	53	26.251	29.620	30.017	1.00	25.22	A
	ATOM 5423	N	HIS	A	62	24.143	29.233	23.623	1.00	22.53	A
20	ATOM 5424	CA	HIS	A	62	22.973	29.778	24.304	1.00	21.30	A
	ATOM 5425	CB	HIS	A	62	22.641	31.181	23.777	1.00	21.36	A
	ATOM 5426	CG	HIS	A	62	22.241	31.212	22.334	1.00	21.08	A
	ATOM 5427	CD2	HIS	A	62	21.074	31.557	21.739	1.00	20.76	A
	ATOM 5428	ND1	HIS	A	62	23.112	30.897	21.314	1.00	21.06	A
25	ATOM 5429	CE1	HIS	A	62	22.502	31.050	20.152	1.00	20.77	A

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	ATOM 5430	NE2	HIS	A	62	21.264	31.449	20.382	1.00	21.11	A
	ATOM 5431	C	HIS	A	62	21.754	28.875	24.145	1.00	20.50	A
	ATOM 5432	O	HIS	A	62	21.812	27.856	23.457	1.00	20.45	A
	ATOM 5433	N	GLN	A	63	20.653	29.279	24.776	1.00	19.38	A
5	ATOM 5434	CA	GLN	A	63	19.395	28.531	24.759	1.00	18.32	A
	ATOM 5435	CB	GLN	A	63	19.006	28.135	23.327	1.00	18.21	A
	ATOM 5436	CG	GLN	A	63	18.351	29.257	22.523	1.00	17.55	A
	ATOM 5437	CD	GLN	A	63	17.052	29.748	23.159	1.00	17.51	A
	ATOM 5438	OE1	GLN	A	63	16.447	29.061	23.990	1.00	16.96	A
10	ATOM 5439	NE2	GLN	A	63	16.614	30.932	22.760	1.00	16.64	A
	ATOM 5440	C	GLN	A	63	19.548	27.295	25.640	1.00	17.51	A
	ATOM 5441	O	GLN	A	63	20.204	26.326	25.262	1.00	17.52	A
	ATOM 5442	N	SER	A	64	18.922	27.343	26.810	1.00	16.62	A
	ATOM 5443	CA	SER	A	64	19.005	26.266	27.787	1.00	16.23	A
15	ATOM 5444	CB	SER	A	64	18.109	26.580	28.994	1.00	15.75	A
	ATOM 5445	OG	SER	A	64	16.739	26.636	28.636	1.00	16.02	A
	ATOM 5446	C	SER	A	64	18.690	24.871	27.264	1.00	16.04	A
	ATOM 5447	O	SER	A	64	19.416	23.927	27.561	1.00	15.93	A
	ATOM 5448	N	LEU	A	65	17.623	24.736	26.484	1.00	15.93	A
20	ATOM 5449	CA	LEU	A	65	17.243	23.426	25.969	1.00	16.08	A
	ATOM 5450	CB	LEU	A	65	15.781	23.445	25.509	1.00	16.21	A
	ATOM 5451	CG	LEU	A	65	14.757	23.960	26.532	1.00	16.82	A
	ATOM 5452	CD1	LEU	A	65	13.348	23.839	25.954	1.00	17.04	A
	ATOM 5453	CD2	LEU	A	65	14.862	23.156	27.831	1.00	16.97	A
25	ATOM 5454	C	LEU	A	65	18.168	22.953	24.846	1.00	16.25	A

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	ATOM 5455	O	LEU A	65	18.403	21.753	24.693	1.00	16.15	A
	ATOM 5662	N	ASP A	93	9.463	20.540	25.416	1.00	15.24	A
	ATOM 5663	CA	ASP A	93	8.886	21.742	24.818	1.00	15.43	A
	ATOM 5664	CB	ASP A	93	8.800	21.598	23.289	1.00	16.54	A
5	ATOM 5665	CG	ASP A	93	10.083	22.013	22.578	1.00	17.29	A
	ATOM 5666	OD1	ASP A	93	10.162	21.833	21.338	1.00	18.80	A
	ATOM 5667	OD2	ASP A	93	11.014	22.527	23.240	1.00	17.97	A
	ATOM 5668	C	ASP A	93	7.496	22.053	25.388	1.00	15.31	A
	ATOM 5669	O	ASP A	93	7.138	23.220	25.568	1.00	15.25	A
10	ATOM 5670	N	THR A	94	6.707	21.016	25.658	1.00	15.02	A
	ATOM 5671	CA	THR A	94	5.371	21.207	26.224	1.00	15.27	A
	ATOM 5672	CB	THR A	94	4.640	19.861	26.399	1.00	15.32	A
	ATOM 5673	OG1	THR A	94	4.193	19.397	25.118	1.00	16.10	A
	ATOM 5674	CG2	THR A	94	3.432	20.011	27.323	1.00	15.76	A
15	ATOM 5675	C	THR A	94	5.483	21.895	27.584	1.00	15.32	A
	ATOM 5676	O	THR A	94	4.756	22.843	27.878	1.00	14.89	A
	ATOM 5677	N	LEU A	95	6.406	21.408	28.407	1.00	15.54	A
	ATOM 5678	CA	LEU A	95	6.615	21.982	29.732	1.00	16.01	A
	ATOM 5679	CB	LEU A	95	7.593	21.115	30.535	1.00	16.19	A
20	ATOM 5680	CG	LEU A	95	7.089	19.738	30.998	1.00	16.12	A
	ATOM 5681	CD1	LEU A	95	8.230	18.966	31.648	1.00	16.47	A
	ATOM 5682	CD2	LEU A	95	5.934	19.903	31.975	1.00	16.46	A
	ATOM 5683	C	LEU A	95	7.167	23.402	29.590	1.00	16.45	A
	ATOM 5684	O	LEU A	95	6.744	24.320	30.296	1.00	16.19	A
25	ATOM 5685	N	ASP A	96	8.112	23.576	28.667	1.00	16.83	A

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	ATOM 5686	CA	ASP	A	96	8.718	24.886	28.435	1.00	17.42	A
	ATOM 5687	CB	ASP	A	96	9.834	24.776	27.388	1.00	17.70	A
	ATOM 5688	CG	ASP	A	96	10.761	25.977	27.397	1.00	18.24	A
	ATOM 5689	OD1	ASP	A	96	11.259	26.318	28.496	1.00	19.16	A
5	ATOM 5690	OD2	ASP	A	96	11.004	26.566	26.314	1.00	17.96	A
	ATOM 5691	C	ASP	A	96	7.670	25.906	27.982	1.00	17.76	A
	ATOM 5692	O	ASP	A	96	7.707	27.074	28.383	1.00	17.65	A
	ATOM 5693	N	ASP	A	97	6.741	25.463	27.140	1.00	18.16	A
	ATOM 5694	CA	ASP	A	97	5.672	26.328	26.642	1.00	18.58	A
10	ATOM 5695	CB	ASP	A	97	4.759	25.559	25.681	1.00	18.77	A
	ATOM 5696	CG	ASP	A	97	5.388	25.333	24.313	1.00	19.31	A
	ATOM 5697	OD1	ASP	A	97	4.838	24.515	23.539	1.00	19.60	A
	ATOM 5698	OD2	ASP	A	97	6.420	25.973	24.007	1.00	19.36	A
	ATOM 5699	C	ASP	A	97	4.820	26.880	27.786	1.00	18.77	A
15	ATOM 5700	O	ASP	A	97	4.480	28.063	27.799	1.00	18.43	A
	ATOM 5701	N	PHE	A	98	4.473	26.017	28.738	1.00	18.98	A
	ATOM 5702	CA	PHE	A	98	3.644	26.427	29.865	1.00	19.59	A
	ATOM 5703	CB	PHE	A	98	3.170	25.208	30.662	1.00	19.85	A
	ATOM 5704	CG	PHE	A	98	2.225	25.554	31.787	1.00	20.49	A
20	ATOM 5705	CD1	PHE	A	98	1.002	26.164	31.520	1.00	20.75	A
	ATOM 5706	CD2	PHE	A	98	2.561	25.279	33.110	1.00	21.00	A
	ATOM 5707	CE1	PHE	A	98	0.126	26.496	32.557	1.00	21.20	A
	ATOM 5708	CE2	PHE	A	98	1.690	25.608	34.156	1.00	20.81	A
	ATOM 5709	CZ	PHE	A	98	0.473	26.216	33.876	1.00	21.25	A
25	ATOM 5710	C	PHE	A	98	4.382	27.373	30.798	1.00	19.70	A

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	ATOM 5711	O	PHE A 98	3.849	28.407	31.193	1.00	19.84	A
	ATOM 5712	N	MET A 99	5.610	27.010	31.148	1.00	19.93	A
	ATOM 5713	CA	MET A 99	6.422	27.834	32.038	1.00	20.62	A
	ATOM 5714	CB	MET A 99	7.759	27.150	32.323	1.00	20.56	A
5	ATOM 5715	CG	MET A 99	7.642	25.794	32.999	1.00	20.77	A
	ATOM 5716	SD	MET A 99	6.765	25.897	34.599	1.00	20.94	A
	ATOM 5717	CE	MET A 99	7.971	26.856	35.571	1.00	21.40	A
	ATOM 5718	C	MET A 99	6.684	29.200	31.418	1.00	21.19	A
	ATOM 5719	O	MET A 99	6.770	30.205	32.123	1.00	20.97	A
10	ATOM 5720	N	SER A 100	6.817	29.232	30.094	1.00	21.87	A
	ATOM 5721	CA	SER A 100	7.088	30.480	29.391	1.00	22.86	A
	ATOM 5722	CB	SER A 100	7.626	30.190	27.986	1.00	22.52	A
	ATOM 5723	OG	SER A 100	8.932	29.641	28.064	1.00	23.15	A
	ATOM 5724	C	SER A 100	5.874	31.400	29.310	1.00	23.42	A
15	ATOM 5725	O	SER A 100	5.999	32.570	28.944	1.00	23.43	A
	ATOM 5726	N	CYS A 101	4.705	30.871	29.656	1.00	24.43	A
	ATOM 5727	CA	CYS A 101	3.470	31.649	29.642	1.00	25.43	A
	ATOM 5728	CB	CYS A 101	2.246	30.732	29.736	1.00	25.71	A
	ATOM 5729	SG	CYS A 101	1.749	29.932	28.189	1.00	27.17	A
20	ATOM 5730	C	CYS A 101	3.427	32.631	30.806	1.00	25.95	A
	ATOM 5731	O	CYS A 101	2.818	33.695	30.704	1.00	25.87	A
	ATOM 5732	N	PHE A 102	4.060	32.272	31.919	1.00	26.64	A
	ATOM 5733	CA	PHE A 102	4.055	33.150	33.084	1.00	27.61	A
	ATOM 5734	CB	PHE A 102	4.567	32.416	34.328	1.00	27.12	A
25	ATOM 5735	CG	PHE A 102	3.679	31.293	34.780	1.00	26.71	A

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	ATOM 5736	CD1	PHE	A	102	3.627	30.100	34.067	1.00	26.53	A
	ATOM 5737	CD2	PHE	A	102	2.904	31.422	35.930	1.00	26.49	A
	ATOM 5738	CE1	PHE	A	102	2.814	29.047	34.495	1.00	26.51	A
	ATOM 5739	CE2	PHE	A	102	2.089	30.378	36.366	1.00	26.35	A
5	ATOM 5740	CZ	PHE	A	102	2.044	29.187	35.648	1.00	26.32	A
	ATOM 5741	C	PHE	A	102	4.896	34.401	32.862	1.00	28.66	A
	ATOM 5742	O	PHE	A	102	6.020	34.328	32.366	1.00	28.59	A
	ATOM 5743	N	PRO	A	103	4.353	35.572	33.228	1.00	29.73	A
	ATOM 5744	CD	PRO	A	103	2.973	35.797	33.697	1.00	29.81	A
10	ATOM 5745	CA	PRO	A	103	5.059	36.846	33.070	1.00	30.81	A
	ATOM 5746	CB	PRO	A	103	3.927	37.865	33.132	1.00	30.54	A
	ATOM 5747	CG	PRO	A	103	3.012	37.251	34.137	1.00	30.22	A
	ATOM 5748	C	PRO	A	103	6.087	37.050	34.183	1.00	31.87	A
	ATOM 5749	O	PRO	A	103	5.896	37.883	35.069	1.00	31.89	A
15	ATOM 5750	N	TRP	A	104	7.173	36.284	34.134	1.00	33.14	A
	ATOM 5751	CA	TRP	A	104	8.218	36.373	35.147	1.00	34.59	A
	ATOM 5752	CB	TRP	A	104	9.315	35.340	34.874	1.00	34.65	A
	ATOM 5753	CG	TRP	A	104	8.796	33.949	34.643	1.00	34.60	A
	ATOM 5754	CD2	TRP	A	104	8.342	33.023	35.639	1.00	34.60	A
20	ATOM 5755	CE2	TRP	A	104	7.930	31.852	34.965	1.00	34.60	A
	ATOM 5756	CE3	TRP	A	104	8.243	33.068	37.038	1.00	34.59	A
	ATOM 5757	CD1	TRP	A	104	8.644	33.320	33.440	1.00	34.55	A
	ATOM 5758	NE1	TRP	A	104	8.126	32.060	33.624	1.00	34.48	A
	ATOM 5759	CZ2	TRP	A	104	7.427	30.736	35.641	1.00	34.52	A
25	ATOM 5760	CZ3	TRP	A	104	7.743	31.959	37.709	1.00	34.54	A

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	ATOM 5761	CH2	TRP	A	104	7.341	30.809	37.009	1.00	34.78	A
	ATOM 5762	C	TRP	A	104	8.837	37.765	35.207	1.00	35.65	A
	ATOM 5763	O	TRP	A	104	9.139	38.270	36.286	1.00	35.74	A
	ATOM 5764	N	ALA	A	105	9.024	38.379	34.044	1.00	37.02	A
5	ATOM 5765	CA	ALA	A	105	9.612	39.712	33.960	1.00	38.45	A
	ATOM 5766	CB	ALA	A	105	10.630	39.762	32.826	1.00	38.40	A
	ATOM 5767	C	ALA	A	105	8.541	40.776	33.743	1.00	39.42	A
	ATOM 5768	O	ALA	A	105	8.562	41.497	32.744	1.00	39.67	A
	ATOM 5769	N	GLU	A	106	7.604	40.871	34.677	1.00	40.55	A
10	ATOM 5770	CA	GLU	A	106	6.536	41.854	34.566	1.00	41.69	A
	ATOM 5771	CB	GLU	A	106	5.178	41.152	34.484	1.00	41.79	A
	ATOM 5772	CG	GLU	A	106	3.996	42.101	34.385	1.00	42.04	A
	ATOM 5773	CD	GLU	A	106	4.119	43.062	33.219	1.00	42.17	A
	ATOM 5774	OE1	GLU	A	106	4.135	42.600	32.059	1.00	42.24	A
15	ATOM 5775	OE2	GLU	A	106	4.207	44.282	33.461	1.00	42.30	A
	ATOM 5776	C	GLU	A	106	6.549	42.817	35.745	1.00	42.38	A
	ATOM 5777	O	GLU	A	106	6.252	42.433	36.877	1.00	42.50	A
	ATOM 5778	N	LYS	A	107	6.902	44.071	35.471	1.00	43.32	A
	ATOM 5779	CA	LYS	A	107	6.949	45.105	36.498	1.00	44.17	A
20	ATOM 5780	CB	LYS	A	107	7.501	46.408	35.916	1.00	44.38	A
	ATOM 5781	CG	LYS	A	107	9.001	46.575	36.067	1.00	44.83	A
	ATOM 5782	CD	LYS	A	107	9.773	45.472	35.376	1.00	45.12	A
	ATOM 5783	CE	LYS	A	107	11.261	45.611	35.654	1.00	45.28	A
	ATOM 5784	NZ	LYS	A	107	11.534	45.551	37.119	1.00	45.38	A
25	ATOM 5785	C	LYS	A	107	5.573	45.364	37.100	1.00	44.67	A

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	ATOM 5786	O	LYS A 107	5.431	45.477	38.318	1.00	44.70	A
	ATOM 5787	N	LYS A 108	4.563	45.460	36.240	1.00	45.16	A
	ATOM 5788	CA	LYS A 108	3.197	45.701	36.688	1.00	45.71	A
	ATOM 5789	CB	LYS A 108	2.268	45.869	35.483	1.00	45.85	A
5	ATOM 5790	CG	LYS A 108	2.686	46.978	34.531	1.00	46.17	A
	ATOM 5791	CD	LYS A 108	1.639	47.224	33.455	1.00	46.42	A
	ATOM 5792	CE	LYS A 108	1.458	46.017	32.549	1.00	46.68	A
	ATOM 5793	NZ	LYS A 108	0.371	46.242	31.554	1.00	46.81	A
	ATOM 5794	C	LYS A 108	2.731	44.533	37.551	1.00	46.00	A
10	ATOM 5795	O	LYS A 108	2.296	43.501	37.038	1.00	45.89	A
	ATOM 5796	N	GLN A 109	2.825	44.704	38.865	1.00	46.38	A
	ATOM 5797	CA	GLN A 109	2.438	43.660	39.809	1.00	46.76	A
	ATOM 5798	CB	GLN A 109	2.710	44.125	41.242	1.00	47.02	A
	ATOM 5799	CG	GLN A 109	4.150	44.545	41.500	1.00	47.38	A
15	ATOM 5800	CD	GLN A 109	5.148	43.428	41.243	1.00	47.66	A
	ATOM 5801	OE1	GLN A 109	5.062	42.353	41.842	1.00	47.81	A
	ATOM 5802	NE2	GLN A 109	6.105	43.679	40.350	1.00	47.68	A
	ATOM 5803	C	GLN A 109	0.977	43.252	39.674	1.00	46.90	A
	ATOM 5804	O	GLN A 109	0.627	42.091	39.890	1.00	46.97	A
20	ATOM 5805	N	ASP A 110	0.127	44.209	39.315	1.00	47.00	A
	ATOM 5806	CA	ASP A 110	-1.301	43.948	39.159	1.00	47.06	A
	ATOM 5807	CB	ASP A 110	-2.046	45.251	38.853	1.00	47.31	A
	ATOM 5808	CG	ASP A 110	-1.945	46.256	39.982	1.00	47.59	A
	ATOM 5809	OD1	ASP A 110	-2.246	45.881	41.136	1.00	47.70	A
25	ATOM 5810	OD2	ASP A 110	-1.571	47.419	39.717	1.00	47.82	A

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	ATOM 5811	C	ASP A 110	-1.584	42.926	38.063	1.00	46.90	A
	ATOM 5812	O	ASP A 110	-2.203	41.891	38.314	1.00	46.87	A
	ATOM 5813	N	VAL A 111	-1.127	43.220	36.850	1.00	46.72	A
	ATOM 5814	CA	VAL A 111	-1.338	42.326	35.719	1.00	46.57	A
5	ATOM 5815	CB	VAL A 111	-0.918	42.999	34.391	1.00	46.71	A
	ATOM 5816	CG1	VAL A 111	0.588	43.192	34.357	1.00	46.96	A
	ATOM 5817	CG2	VAL A 111	-1.378	42.160	33.213	1.00	46.81	A
	ATOM 5818	C	VAL A 111	-0.550	41.029	35.894	1.00	46.33	A
	ATOM 5819	O	VAL A 111	-0.967	39.970	35.426	1.00	46.33	A
10	ATOM 5820	N	LYS A 112	0.588	41.117	36.573	1.00	45.98	A
	ATOM 5821	CA	LYS A 112	1.427	39.949	36.810	1.00	45.58	A
	ATOM 5822	CB	LYS A 112	2.772	40.383	37.397	1.00	45.70	A
	ATOM 5823	CG	LYS A 112	3.753	39.245	37.630	1.00	45.79	A
	ATOM 5824	CD	LYS A 112	5.070	39.765	38.187	1.00	45.95	A
15	ATOM 5825	CE	LYS A 112	6.087	38.646	38.340	1.00	45.99	A
	ATOM 5826	NZ	LYS A 112	5.582	37.571	39.237	1.00	46.23	A
	ATOM 5827	C	LYS A 112	0.732	38.985	37.768	1.00	45.31	A
	ATOM 5828	O	LYS A 112	0.597	37.793	37.481	1.00	45.18	A
	ATOM 5829	N	GLU A 113	0.290	39.515	38.904	1.00	44.80	A
20	ATOM 5830	CA	GLU A 113	-0.390	38.718	39.920	1.00	44.37	A
	ATOM 5831	CB	GLU A 113	-0.817	39.615	41.089	1.00	44.56	A
	ATOM 5832	CG	GLU A 113	-1.246	38.872	42.346	1.00	44.72	A
	ATOM 5833	CD	GLU A 113	-0.069	38.326	43.135	1.00	44.84	A
	ATOM 5834	OE1	GLU A 113	0.653	37.451	42.611	1.00	44.74	A
25	ATOM 5835	OE2	GLU A 113	0.138	38.780	44.281	1.00	44.95	A

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	ATOM 5836	C	GLU A 113	-1.620	38.044	39.316	1.00	43.91	A
	ATOM 5837	O	GLU A 113	-1.907	36.878	39.594	1.00	43.88	A
	ATOM 5838	N	GLN A 114	-2.343	38.789	38.486	1.00	43.23	A
	ATOM 5839	CA	GLN A 114	-3.545	38.276	37.843	1.00	42.55	A
5	ATOM 5840	CB	GLN A 114	-4.243	39.392	37.063	1.00	43.01	A
	ATOM 5841	CG	GLN A 114	-5.502	38.952	36.330	1.00	43.48	A
	ATOM 5842	CD	GLN A 114	-6.660	38.643	37.266	1.00	43.87	A
	ATOM 5843	OE1	GLN A 114	-7.716	38.182	36.831	1.00	44.27	A
	ATOM 5844	NE2	GLN A 114	-6.469	38.902	38.556	1.00	44.00	A
10	ATOM 5845	C	GLN A 114	-3.241	37.115	36.902	1.00	41.82	A
	ATOM 5846	O	GLN A 114	-3.862	36.058	36.993	1.00	41.68	A
	ATOM 5847	N	MET A 115	-2.287	37.318	35.999	1.00	40.95	A
	ATOM 5848	CA	MET A 115	-1.914	36.286	35.039	1.00	40.08	A
	ATOM 5849	CB	MET A 115	-0.823	36.806	34.096	1.00	40.62	A
15	ATOM 5850	CG	MET A 115	-1.283	37.947	33.197	1.00	41.32	A
	ATOM 5851	SD	MET A 115	-0.084	38.396	31.912	1.00	42.25	A
	ATOM 5852	CE	MET A 115	0.892	39.641	32.771	1.00	42.06	A
	ATOM 5853	C	MET A 115	-1.451	34.995	35.711	1.00	39.18	A
	ATOM 5854	O	MET A 115	-1.750	33.899	35.233	1.00	38.94	A
20	ATOM 5855	N	PHE A 116	-0.723	35.120	36.817	1.00	38.04	A
	ATOM 5856	CA	PHE A 116	-0.246	33.943	37.535	1.00	37.08	A
	ATOM 5857	CB	PHE A 116	0.632	34.347	38.725	1.00	36.65	A
	ATOM 5858	CG	PHE A 116	2.104	34.250	38.453	1.00	36.16	A
	ATOM 5859	CD1	PHE A 116	2.707	35.072	37.509	1.00	36.15	A
25	ATOM 5860	CD2	PHE A 116	2.887	33.323	39.130	1.00	36.09	A

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	ATOM 5861	CE1 PHE A 116	4.070	34.970	37.241	1.00	36.00	A
	ATOM 5862	CE2 PHE A 116	4.250	33.213	38.870	1.00	36.03	A
	ATOM 5863	CZ PHE A 116	4.841	34.038	37.923	1.00	36.03	A
	ATOM 5864	C PHE A 116	-1.406	33.087	38.033	1.00	36.66	A
5	ATOM 5865	O PHE A 116	-1.454	31.882	37.782	1.00	36.40	A
	ATOM 6152	N TYR A 152	13.399	17.626	33.588	1.00	17.13	A
	ATOM 6153	CA TYR A 152	12.704	18.883	33.352	1.00	16.94	A
	ATOM 6154	CB TYR A 152	12.549	19.144	31.854	1.00	17.23	A
	ATOM 6155	CG TYR A 152	12.463	20.619	31.522	1.00	17.59	A
10	ATOM 6156	CD1 TYR A 152	13.414	21.519	32.010	1.00	17.83	A
	ATOM 6157	CE1 TYR A 152	13.368	22.871	31.673	1.00	18.02	A
	ATOM 6158	CD2 TYR A 152	11.459	21.111	30.693	1.00	17.66	A
	ATOM 6159	CE2 TYR A 152	11.407	22.460	30.349	1.00	17.94	A
	ATOM 6160	CZ TYR A 152	12.363	23.331	30.837	1.00	18.06	A
15	ATOM 6161	OH TYR A 152	12.339	24.652	30.461	1.00	18.13	A
	ATOM 6162	C TYR A 152	11.342	18.931	34.031	1.00	17.03	A
	ATOM 6163	O TYR A 152	10.893	19.996	34.459	1.00	16.79	A
	ATOM 6164	N TRP A 153	10.684	17.780	34.127	1.00	16.68	A
	ATOM 6165	CA TRP A 153	9.391	17.714	34.782	1.00	16.70	A
20	ATOM 6166	CB TRP A 153	8.792	16.311	34.662	1.00	17.07	A
	ATOM 6167	CG TRP A 153	7.822	16.001	35.761	1.00	18.05	A
	ATOM 6168	CD2 TRP A 153	6.615	16.708	36.066	1.00	18.42	A
	ATOM 6169	CE2 TRP A 153	6.049	16.095	37.206	1.00	18.78	A
	ATOM 6170	CE3 TRP A 153	5.956	17.800	35.488	1.00	18.93	A
25	ATOM 6171	CD1 TRP A 153	7.936	15.014	36.699	1.00	18.52	A

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	ATOM 6172	NE1	TRP	A	153	6.874	15.065	37.570	1.00	18.65	A
	ATOM 6173	CZ2	TRP	A	153	4.852	16.540	37.781	1.00	18.98	A
	ATOM 6174	CZ3	TRP	A	153	4.761	18.245	36.063	1.00	19.09	A
	ATOM 6175	CH2	TRP	A	153	4.225	17.613	37.198	1.00	18.95	A
5	ATOM 6176	C	TRP	A	153	9.578	18.055	36.253	1.00	16.19	A
	ATOM 6177	O	TRP	A	153	8.844	18.868	36.804	1.00	16.11	A
	ATOM 6178	N	GLU	A	154	10.571	17.429	36.879	1.00	15.99	A
	ATOM 6179	CA	GLU	A	154	10.850	17.652	38.301	1.00	15.99	A
	ATOM 6180	CB	GLU	A	154	11.985	16.725	38.759	1.00	16.41	A
10	ATOM 6181	CG	GLU	A	154	12.159	16.644	40.282	1.00	17.45	A
	ATOM 6182	CD	GLU	A	154	12.954	17.795	40.864	1.00	17.87	A
	ATOM 6183	OE1	GLU	A	154	12.895	18.000	42.103	1.00	18.47	A
	ATOM 6184	OE2	GLU	A	154	13.648	18.489	40.093	1.00	18.04	A
	ATOM 6185	C	GLU	A	154	11.208	19.112	38.564	1.00	15.58	A
15	ATOM 6186	O	GLU	A	154	10.793	19.697	39.568	1.00	15.32	A
	ATOM 6187	N	ILE	A	155	11.973	19.694	37.647	1.00	14.97	A
	ATOM 6188	CA	ILE	A	155	12.391	21.088	37.747	1.00	14.96	A
	ATOM 6189	CB	ILE	A	155	13.460	21.401	36.665	1.00	14.64	A
	ATOM 6190	CG2	ILE	A	155	13.621	22.906	36.479	1.00	14.51	A
20	ATOM 6191	CG1	ILE	A	155	14.779	20.722	37.054	1.00	14.76	A
	ATOM 6192	CD1	ILE	A	155	15.871	20.787	35.989	1.00	14.27	A
	ATOM 6193	C	ILE	A	155	11.207	22.044	37.609	1.00	15.18	A
	ATOM 6194	O	ILE	A	155	11.032	22.952	38.425	1.00	15.10	A
	ATOM 6195	N	CYS	A	156	10.394	21.840	36.574	1.00	15.13	A
25	ATOM 6196	CA	CYS	A	156	9.225	22.688	36.351	1.00	15.67	A

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	ATOM 6197	CB	CYS A 156	8.573	22.365	34.998	1.00	15.61	A
	ATOM 6198	SG	CYS A 156	9.519	22.879	33.537	1.00	16.74	A
	ATOM 6199	C	CYS A 156	8.175	22.557	37.462	1.00	15.81	A
	ATOM 6200	O	CYS A 156	7.612	23.558	37.904	1.00	15.91	A
5	ATOM 6201	N	SER A 157	7.904	21.331	37.905	1.00	15.84	A
	ATOM 6202	CA	SER A 157	6.908	21.113	38.954	1.00	16.04	A
	ATOM 6203	CB	SER A 157	6.614	19.614	39.117	1.00	15.82	A
	ATOM 6204	OG	SER A 157	7.799	18.879	39.353	1.00	15.23	A
	ATOM 6205	C	SER A 157	7.375	21.713	40.279	1.00	16.34	A
10	ATOM 6206	O	SER A 157	6.566	22.205	41.075	1.00	16.25	A
	ATOM 6207	N	THR A 158	8.681	21.678	40.519	1.00	16.57	A
	ATOM 6208	CA	THR A 158	9.218	22.252	41.750	1.00	17.18	A
	ATOM 6209	CB	THR A 158	10.756	22.149	41.796	1.00	17.24	A
	ATOM 6210	OG1	THR A 158	11.129	20.790	42.058	1.00	17.94	A
15	ATOM 6211	CG2	THR A 158	11.324	23.039	42.895	1.00	17.40	A
	ATOM 6212	C	THR A 158	8.807	23.721	41.862	1.00	17.28	A
	ATOM 6213	O	THR A 158	8.266	24.154	42.884	1.00	17.37	A
	ATOM 6214	N	THR A 159	9.056	24.484	40.805	1.00	17.51	A
	ATOM 6215	CA	THR A 159	8.705	25.900	40.790	1.00	17.92	A
20	ATOM 6216	CB	THR A 159	9.303	26.594	39.543	1.00	17.65	A
	ATOM 6217	OG1	THR A 159	10.730	26.596	39.653	1.00	17.96	A
	ATOM 6218	CG2	THR A 159	8.812	28.033	39.421	1.00	18.36	A
	ATOM 6219	C	THR A 159	7.193	26.107	40.836	1.00	17.91	A
	ATOM 6220	O	THR A 159	6.702	26.981	41.554	1.00	18.18	A
25	ATOM 6221	N	LEU A 160	6.446	25.307	40.084	1.00	18.04	A

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	ATOM 6222	CA	LEU A 160	4.995	25.448	40.098	1.00	18.10	A
	ATOM 6223	CB	LEU A 160	4.350	24.485	39.102	1.00	18.30	A
	ATOM 6224	CG	LEU A 160	4.599	24.829	37.627	1.00	18.44	A
	ATOM 6225	CD1	LEU A 160	3.998	23.744	36.741	1.00	18.61	A
5	ATOM 6226	CD2	LEU A 160	3.995	26.185	37.298	1.00	18.31	A
	ATOM 6227	C	LEU A 160	4.445	25.190	41.500	1.00	18.29	A
	ATOM 6228	O	LEU A 160	3.524	25.874	41.939	1.00	18.04	A
	ATOM 6229	N	LEU A 161	5.014	24.209	42.199	1.00	18.58	A
	ATOM 6230	CA	LEU A 161	4.562	23.867	43.554	1.00	18.65	A
10	ATOM 6231	CB	LEU A 161	5.288	22.617	44.061	1.00	18.76	A
	ATOM 6232	CG	LEU A 161	4.830	21.269	43.494	1.00	18.94	A
	ATOM 6233	CD1	LEU A 161	5.881	20.206	43.761	1.00	18.87	A
	ATOM 6234	CD2	LEU A 161	3.494	20.881	44.115	1.00	18.81	A
	ATOM 6235	C	LEU A 161	4.769	25.009	44.545	1.00	18.70	A
15	ATOM 6236	O	LEU A 161	4.100	25.078	45.580	1.00	18.70	A
	ATOM 6237	N	VAL A 162	5.713	25.892	44.242	1.00	18.91	A
	ATOM 6238	CA	VAL A 162	5.982	27.038	45.111	1.00	19.05	A
	ATOM 6239	CB	VAL A 162	7.268	27.775	44.679	1.00	18.98	A
	ATOM 6240	CG1	VAL A 162	7.376	29.108	45.403	1.00	19.21	A
20	ATOM 6241	CG2	VAL A 162	8.485	26.911	44.990	1.00	18.86	A
	ATOM 6242	C	VAL A 162	4.807	28.012	45.079	1.00	19.45	A
	ATOM 6243	O	VAL A 162	4.496	28.669	46.076	1.00	19.46	A
	ATOM 6244	N	PHE A 163	4.144	28.096	43.932	1.00	19.57	A
	ATOM 6245	CA	PHE A 163	3.013	28.998	43.797	1.00	20.03	A
25	ATOM 6246	CB	PHE A 163	3.087	29.734	42.458	1.00	20.31	A

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	ATOM 6247	CG	PHE A 163	4.337	30.550	42.291	1.00	20.50	A
	ATOM 6248	CD1	PHE A 163	5.466	29.999	41.696	1.00	20.62	A
	ATOM 6249	CD2	PHE A 163	4.403	31.856	42.771	1.00	20.68	A
	ATOM 6250	CE1	PHE A 163	6.644	30.732	41.581	1.00	20.55	A
5	ATOM 6251	CE2	PHE A 163	5.578	32.598	42.661	1.00	20.66	A
	ATOM 6252	CZ	PHE A 163	6.701	32.032	42.064	1.00	20.63	A
	ATOM 6253	C	PHE A 163	1.669	28.302	43.933	1.00	20.28	A
	ATOM 6254	O	PHE A 163	0.664	28.948	44.218	1.00	20.48	A
	ATOM 6528	N	THR A 197	16.338	29.399	46.423	1.00	26.20	A
10	ATOM 6529	CA	THR A 197	15.751	30.609	45.863	1.00	25.74	A
	ATOM 6530	CB	THR A 197	16.490	31.036	44.577	1.00	25.61	A
	ATOM 6531	OG1	THR A 197	16.472	29.955	43.637	1.00	25.05	A
	ATOM 6532	CG2	THR A 197	17.930	31.404	44.885	1.00	25.60	A
	ATOM 6533	C	THR A 197	14.275	30.422	45.534	1.00	25.48	A
15	ATOM 6534	O	THR A 197	13.779	29.297	45.478	1.00	25.55	A
	ATOM 6535	N	LYS A 198	13.579	31.533	45.321	1.00	25.39	A
	ATOM 6536	CA	LYS A 198	12.158	31.503	44.987	1.00	25.33	A
	ATOM 6537	CB	LYS A 198	11.588	32.923	44.977	1.00	25.43	A
	ATOM 6538	CG	LYS A 198	10.103	32.992	44.646	1.00	25.92	A
20	ATOM 6539	CD	LYS A 198	9.614	34.427	44.597	1.00	26.17	A
	ATOM 6540	CE	LYS A 198	8.186	34.502	44.089	1.00	26.49	A
	ATOM 6541	NZ	LYS A 198	7.712	35.915	43.956	1.00	26.69	A
	ATOM 6542	C	LYS A 198	11.943	30.855	43.621	1.00	25.18	A
	ATOM 6543	O	LYS A 198	11.110	29.962	43.473	1.00	24.95	A
25	ATOM 6544	N	LEU A 199	12.699	31.313	42.628	1.00	25.13	A

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	ATOM 6545	CA	LEU A 199	12.595	30.781	41.270	1.00	25.12	A
	ATOM 6546	CB	LEU A 199	12.408	31.930	40.275	1.00	25.36	A
	ATOM 6547	CG	LEU A 199	10.969	32.324	39.926	1.00	25.73	A
	ATOM 6548	CD1	LEU A 199	10.105	32.362	41.171	1.00	25.91	A
5	ATOM 6549	CD2	LEU A 199	10.981	33.665	39.212	1.00	25.98	A
	ATOM 6550	C	LEU A 199	13.812	29.952	40.870	1.00	25.09	A
	ATOM 6551	O	LEU A 199	14.823	29.989	41.603	1.00	24.71	A
	ATOM 6552	OXT	LEU A 199	13.742	29.281	39.817	1.00	24.81	A
	ATOM 6613	N1	GSH H 200	14.696	30.844	25.962	1.00	23.65	H
10	ATOM 6614	CA1	GSH H 200	16.039	31.001	26.524	1.00	23.55	H
	ATOM 6615	C1	GSH H 200	16.542	29.694	27.171	1.00	23.17	H
	ATOM 6616	O11	GSH H 200	15.739	28.768	27.396	1.00	22.46	H
	ATOM 6617	O12	GSH H 200	17.802	29.693	27.562	1.00	22.86	H
	ATOM 6618	CB1	GSH H 200	15.985	32.066	27.622	1.00	23.81	H
15	ATOM 6619	CG1	GSH H 200	15.892	33.498	27.090	1.00	24.34	H
	ATOM 6620	CD1	GSH H 200	15.490	34.394	28.280	1.00	23.98	H
	ATOM 6621	OE1	GSH H 200	14.442	35.015	28.215	1.00	24.41	H
	ATOM 6622	N2	GSH H 200	16.359	34.466	29.315	1.00	24.28	H
	ATOM 6623	CA2	GSH H 200	16.110	35.405	30.441	1.00	24.46	H
20	ATOM 6624	C2	GSH H 200	16.959	36.558	30.276	1.00	24.90	H
	ATOM 6625	O2	GSH H 200	18.145	36.447	29.952	1.00	24.83	H
	ATOM 6626	CB2	GSH H 200	16.495	34.762	31.809	1.00	24.14	H
	ATOM 6627	SG2	GSH H 200	15.212	33.684	32.529	1.00	23.62	H
	ATOM 6628	N3	GSH H 200	16.418	37.764	30.605	1.00	25.69	H
25	ATOM 6629	CA3	GSH H 200	17.234	39.007	30.688	1.00	26.56	H

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	ATOM 6630	C3	GSH H 200	16.858	39.970	29.572	1.00	27.05	H
	ATOM 6631	O31	GSH H 200	17.544	41.013	29.478	1.00	27.21	H
	ATOM 6632	O32	GSH H 200	15.926	39.647	28.800	1.00	27.38	H
	ATOM 6708	C1	U44 X 201	12.551	37.412	34.770	1.00	51.36	X
5	ATOM 6709	C2	U44 X 201	12.942	38.049	36.088	1.00	51.45	X
	ATOM 6710	C3	U44 X 201	13.074	36.818	37.021	1.00	51.46	X
	ATOM 6711	C4	U44 X 201	13.773	35.785	36.065	1.00	51.25	X
	ATOM 6712	C5	U44 X 201	13.862	36.633	34.758	1.00	51.32	X
	ATOM 6713	C7	U44 X 201	14.906	37.744	34.890	1.00	51.38	X
10	ATOM 6714	O6	U44 X 201	14.219	38.627	35.787	1.00	51.43	X
	ATOM 6715	C14	U44 X 201	13.023	34.496	35.785	1.00	50.82	X
	ATOM 6716	C16	U44 X 201	13.358	33.226	36.116	1.00	50.17	X
	ATOM 6717	C18	U44 X 201	12.548	31.983	35.806	1.00	49.75	X
	ATOM 6718	C20	U44 X 201	12.422	31.711	34.291	1.00	49.34	X
15	ATOM 6719	C21	U44 X 201	11.452	30.558	33.949	1.00	48.88	X
	ATOM 6720	C24	U44 X 201	12.111	29.171	34.031	1.00	48.50	X
	ATOM 6721	C27	U44 X 201	11.176	28.042	33.569	1.00	48.26	X
	ATOM 6722	C30	U44 X 201	11.730	26.655	33.911	1.00	47.93	X
	ATOM 6723	O36	U44 X 201	11.255	32.146	36.348	1.00	49.97	X
20	ATOM 6724	C39	U44 X 201	13.871	37.120	38.326	1.00	51.81	X
	ATOM 6725	C41	U44 X 201	13.309	36.423	39.545	1.00	52.19	X
	ATOM 6726	C44	U44 X 201	12.673	36.957	40.612	1.00	52.52	X
	ATOM 6727	C46	U44 X 201	12.354	38.413	40.860	1.00	52.74	X
	ATOM 6728	C48	U44 X 201	11.089	38.600	41.702	1.00	52.91	X
25	ATOM 6729	C51	U44 X 201	10.411	39.953	41.420	1.00	53.03	X

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	ATOM 6730	C54 U44 X 201	8.878	39.832	41.396	1.00	53.12	X
	ATOM 6731	O57 U44 X 201	8.298	41.019	41.144	1.00	53.23	X
	ATOM 6732	O58 U44 X 201	8.266	38.823	41.572	1.00	53.07	X
	ATOM 6734	CA+2 CA2 M 901	9.824	26.883	22.168	1.00	37.63	M
5	ATOM 6747	OH2 WAT S 53	10.720	26.574	23.734	1.00	13.42	S
	ATOM 6748	OH2 WAT S 54	8.700	27.621	24.867	1.00	30.29	S
	ATOM 6749	OH2 WAT S 55	11.193	25.711	20.926	1.00	38.39	S
	ATOM 6750	OH2 WAT S 56	8.649	29.181	22.554	1.00	40.32	S
	ATOM 6751	OH2 WAT S 57	8.686	24.965	22.598	1.00	24.31	S
10	ATOM 6753	OH2 WAT S 59	12.609	27.997	22.910	1.00	26.01	S
	ATOM 6754	OH2 WAT S 60	16.147	26.525	24.446	1.00	13.92	S
	ATOM 6805	OH2 WAT S 119	15.889	24.704	33.708	1.00	12.20	S
	ATOM 6817	OH2 WAT S 131	21.842	34.840	24.519	1.00	17.76	S
	ATOM 6831	OH2 WAT S 145	13.761	25.970	37.415	1.00	14.51	S
15	ATOM 6838	OH2 WAT S 152	19.797	31.378	26.404	1.00	15.01	S
	ATOM 6840	OH2 WAT S 154	17.705	34.244	22.558	1.00	19.55	S
	ATOM 6862	OH2 WAT S 176	15.045	34.087	23.449	1.00	22.78	S
	ATOM 6865	OH2 WAT S 179	24.231	27.246	21.186	1.00	17.23	S
	ATOM 6868	OH2 WAT S 182	15.019	25.681	30.985	1.00	20.42	S
20	ATOM 6880	OH2 WAT S 194	18.957	28.395	43.148	1.00	25.25	S
	ATOM 6884	OH2 WAT S 198	29.524	31.402	30.656	1.00	21.38	S
	ATOM 6891	OH2 WAT S 205	12.982	24.357	39.397	1.00	27.06	S
	ATOM 6911	OH2 WAT S 225	20.243	26.057	41.600	1.00	17.45	S
	ATOM 6915	OH2 WAT S 229	13.072	28.340	28.775	1.00	23.00	S
25	ATOM 6920	OH2 WAT S 234	14.180	35.687	21.027	1.00	19.10	S

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	ATOM 6925	OH2 WAT S 239	16.432	26.840	45.110	1.00	20.16	S
	ATOM 6963	OH2 WAT S 277	9.688	38.330	46.556	1.00	22.33	S
	ATOM 6971	OH2 WAT S 285	14.267	37.710	28.281	1.00	27.08	S
	ATOM 6979	OH2 WAT S 293	14.265	21.922	40.759	1.00	26.98	S
5	ATOM 7003	OH2 WAT S 318	14.285	33.826	42.961	1.00	21.76	S
	ATOM 7004	OH2 WAT S 319	18.057	40.943	23.782	1.00	35.39	S
	ATOM 7031	OH2 WAT S 349	17.934	35.785	45.678	1.00	28.45	S
	ATOM 7060	OH2 WAT S 383	19.852	33.145	23.977	1.00	20.17	S
	ATOM 7071	OH2 WAT S 394	11.887	37.040	22.324	1.00	21.27	S
10	ATOM 7083	OH2 WAT S 407	13.826	35.564	25.333	1.00	32.89	S
	ATOM 7091	OH2 WAT S 415	12.313	24.839	23.220	1.00	28.21	S
	ATOM 7128	OH2 WAT S 454	4.663	29.761	25.692	1.00	33.93	S
	ATOM 7130	OH2 WAT S 456	21.062	36.900	40.187	1.00	38.49	S
	ATOM 7141	OH2 WAT S 467	16.347	39.603	43.840	1.00	38.49	S
15	ATOM 7172	OH2 WAT S 501	16.867	34.824	43.591	1.00	33.65	S
	ATOM 7178	OH2 WAT S 508	13.919	42.210	21.359	1.00	42.62	S
	ATOM 7203	OH2 WAT S 535	24.768	29.671	36.812	1.00	21.16	S
	ATOM 7278	OH2 WAT S 624	9.448	41.034	37.745	1.00	45.08	S
	ATOM 7311	OH2 WAT S 661	10.417	43.064	40.521	1.00	48.24	S
20	ATOM 7338	OH2 WAT S 690	4.520	39.297	24.898	1.00	35.89	S
	ATOM 7357	OH2 WAT S 710	11.398	29.430	37.336	1.00	55.44	S
	ATOM 7372	OH2 WAT S 725	29.681	36.478	31.530	1.00	46.34	S
	ATOM 7377	OH2 WAT S 730	22.836	45.124	25.173	1.00	37.85	S
	ATOM 7421	OH2 WAT S 777	9.127	46.643	25.394	1.00	40.66	S
25	ATOM 7479	OH2 WAT S 842	17.602	38.997	20.277	1.00	32.58	S

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ATOM 7534 OH2 WAT S 900 16.041 43.445 43.323 1.00 38.46 S
ATOM 7540 OH2 WAT S 906 21.141 36.590 45.196 1.00 37.28 S
ATOM 7541 OH2 WAT S 907 25.332 34.472 44.401 1.00 47.03 S
ATOM 7551 OH2 WAT S 917 16.854 44.879 23.884 1.00 42.35 S
5 ATOM 7554 OH2 WAT S 920 8.757 33.269 28.017 1.00 43.49 S
ATOM 7647 OH2 WAT T 22 14.573 42.133 41.410 1.00 38.47 T
ATOM 7652 OH2 WAT T 27 19.585 45.803 29.005 1.00 44.65 T
ATOM 7655 OH2 WAT T 30 17.572 36.979 22.241 1.00 37.46 T
ATOM 7658 OH2 WAT T 35 6.940 39.912 44.003 1.00 34.76 T

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Table 6

Three-dimensional structural coordinate of the complex of
human hematopoietic PGDS with magnesium, glutathione and
9,11-dideoxy -9 α ,11 α -epoxymethanoprostaglandine F_{2 α} (U44)

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ATOM 4966 N TYR A 8 -24.963 2.816 34.571 1.00 17.22 A N
ATOM 4967 CA TYR A 8 -23.542 2.548 34.744 1.00 17.23 A C
ATOM 4968 CB TYR A 8 -22.782 3.882 34.816 1.00 18.03 A C
ATOM 4969 CG TYR A 8 -21.275 3.759 34.770 1.00 16.45 A C
20 ATOM 4970 CD1 TYR A 8 -20.632 3.243 33.642 1.00 15.64 A C
ATOM 4971 CE1 TYR A 8 -19.248 3.117 33.595 1.00 15.32 A C
ATOM 4972 CD2 TYR A 8 -20.491 4.152 35.854 1.00 15.73 A C
ATOM 4973 CE2 TYR A 8 -19.101 4.032 35.821 1.00 16.61 A C
ATOM 4974 CZ TYR A 8 -18.486 3.511 34.688 1.00 15.90 A C
25 ATOM 4975 OH TYR A 8 -17.116 3.369 34.652 1.00 14.22 A O

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	ATOM 4976	C	TYR	A	8	-23.334	1.757	36.033	1.00	18.22	A	C
	ATOM 4977	O	TYR	A	8	-24.286	1.500	36.765	1.00	18.88	A	O
	ATOM 4978	N	PHE	A	9	-22.090	1.365	36.297	1.00	19.45	A	N
	ATOM 4979	CA	PHE	A	9	-21.755	0.631	37.511	1.00	18.46	A	C
5	ATOM 4980	CB	PHE	A	9	-20.326	0.086	37.442	1.00	20.61	A	C
	ATOM 4981	CG	PHE	A	9	-20.127	-0.989	36.416	1.00	21.63	A	C
	ATOM 4982	CD1	PHE	A	9	-19.215	-0.817	35.380	1.00	23.34	A	C
	ATOM 4983	CD2	PHE	A	9	-20.830	-2.184	36.497	1.00	23.29	A	C
	ATOM 4984	CE1	PHE	A	9	-19.003	-1.824	34.439	1.00	23.36	A	C
10	ATOM 4985	CE2	PHE	A	9	-20.627	-3.197	35.564	1.00	23.79	A	C
	ATOM 4986	CZ	PHE	A	9	-19.710	-3.016	34.531	1.00	24.43	A	C
	ATOM 4987	C	PHE	A	9	-21.844	1.610	38.669	1.00	19.26	A	C
	ATOM 4988	O	PHE	A	9	-22.025	2.812	38.457	1.00	18.28	A	O
	ATOM 4989	N	ASN	A	10	-21.720	1.102	39.892	1.00	19.26	A	N
15	ATOM 4990	CA	ASN	A	10	-21.768	1.967	41.062	1.00	20.39	A	C
	ATOM 4991	CB	ASN	A	10	-22.307	1.229	42.289	1.00	19.56	A	C
	ATOM 4992	CG	ASN	A	10	-22.172	2.053	43.558	1.00	20.32	A	C
	ATOM 4993	OD1	ASN	A	10	-22.514	3.239	43.580	1.00	20.34	A	O
	ATOM 4994	ND2	ASN	A	10	-21.675	1.432	44.618	1.00	19.12	A	N
20	ATOM 4995	C	ASN	A	10	-20.382	2.503	41.374	1.00	20.96	A	C
	ATOM 4996	O	ASN	A	10	-19.672	1.971	42.228	1.00	20.75	A	O
	ATOM 4997	N	MET	A	11	-19.998	3.547	40.651	1.00	21.28	A	N
	ATOM 4998	CA	MET	A	11	-18.712	4.202	40.837	1.00	21.14	A	C
	ATOM 4999	CB	MET	A	11	-17.558	3.255	40.479	1.00	24.46	A	C
25	ATOM 5000	CG	MET	A	11	-17.593	2.644	39.097	1.00	28.37	A	C

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	ATOM 5001	SD	MET	A	11	-16.405	1.269	38.962	1.00	31.57	A	S
	ATOM 5002	CE	MET	A	11	-17.463	-0.102	39.381	1.00	33.95	A	C
	ATOM 5003	C	MET	A	11	-18.690	5.449	39.971	1.00	17.84	A	C
	ATOM 5004	O	MET	A	11	-19.542	5.614	39.102	1.00	17.49	A	O
5	ATOM 5005	N	ARG	A	12	-17.747	6.346	40.230	1.00	15.79	A	N
	ATOM 5006	CA	ARG	A	12	-17.652	7.567	39.440	1.00	14.18	A	C
	ATOM 5007	CB	ARG	A	12	-16.607	8.512	40.040	1.00	13.02	A	C
	ATOM 5008	CG	ARG	A	12	-16.888	8.917	41.491	1.00	15.40	A	C
	ATOM 5009	CD	ARG	A	12	-15.857	9.928	41.986	1.00	14.27	A	C
10	ATOM 5010	NE	ARG	A	12	-14.488	9.425	41.848	1.00	15.20	A	N
	ATOM 5011	CZ	ARG	A	12	-13.945	8.494	42.627	1.00	14.91	A	C
	ATOM 5012	NH1	ARG	A	12	-14.649	7.957	43.613	1.00	15.94	A	N
	ATOM 5013	NH2	ARG	A	2	-12.700	8.094	42.416	1.00	14.17	A	N
	ATOM 5014	C	ARG	A	12	-17.258	7.170	38.020	1.00	14.06	A	C
15	ATOM 5015	O	ARG	A	12	-18.014	7.373	37.076	1.00	12.72	A	O
	ATOM 5016	N	GLY	A	13	-16.067	6.598	37.889	1.00	13.50	A	N
	ATOM 5017	CA	GLY	A	13	-15.581	6.151	36.598	1.00	13.43	A	C
	ATOM 5018	C	GLY	A	13	-15.880	7.031	35.397	1.00	11.86	A	C
	ATOM 5019	O	GLY	A	13	-15.654	8.240	35.420	1.00	10.45	A	O
20	ATOM 5020	N	ARG	A	14	-16.398	6.406	34.343	1.00	11.37	A	N
	ATOM 5021	CA	ARG	A	14	-16.708	7.100	33.096	1.00	12.46	A	C
	ATOM 5022	CB	ARG	A	14	-16.606	6.111	31.928	1.00	11.33	A	C
	ATOM 5023	CG	ARG	A	14	-15.177	5.691	31.628	1.00	13.46	A	C
	ATOM 5024	CD	ARG	A	14	-15.077	4.572	30.606	1.00	17.48	A	C
25	ATOM 5025	NE	ARG	A	14	-13.738	4.519	30.019	1.00	20.64	A	N

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	ATOM 5026 CZ ARG A 14	-12.890	3.499	30.132	1.00	22.84	A C
	ATOM 5027 NH1 ARG A 14	-13.224	2.410	30.817	1.00	23.14	A N
	ATOM 5028 NH2 ARG A 14	-11.696	3.575	29.559	1.00	23.88	A N
	ATOM 5029 C ARG A 14	-18.058	7.809	33.049	1.00	11.90	A C
5	ATOM 5030 O ARG A 14	-18.353	8.511	32.087	1.00	12.49	A O
	ATOM 5031 N ALA A 15	-18.871	7.637	34.084	1.00	12.15	A N
	ATOM 5032 CA ALA A 15	-20.190	8.263	34.118	1.00	12.60	A C
	ATOM 5033 CB ALA A 15	-21.206	7.305	34.762	1.00	13.45	A C
	ATOM 5034 C ALA A 15	-20.199	9.592	34.866	1.00	11.68	A C
10	ATOM 5035 O ALA A 15	-21.085	10.423	34.658	1.00	11.89	A O
	ATOM 5036 N GLU A 16	-19.209	9.795	35.727	1.00	13.81	A N
	ATOM 5037 CA GLU A 16	-19.141	11.007	36.534	1.00	13.28	A C
	ATOM 5038 CB GLU A 16	-17.877	10.986	37.399	1.00	12.67	A C
	ATOM 5039 CG GLU A 16	-17.971	11.841	38.672	1.00	13.36	A C
15	ATOM 5040 CD GLU A 16	-19.146	11.457	39.575	1.00	13.41	A C
	ATOM 5041 OE1 GLU A 16	-19.695	10.345	39.422	1.00	12.47	A O
	ATOM 5042 OE2 GLU A 16	-19.512	12.266	40.452	1.00	14.67	A O
	ATOM 5043 C GLU A 16	-19.216	12.314	35.748	1.00	13.25	A C
	ATOM 5044 O GLU A 16	-19.903	13.245	36.167	1.00	11.55	A O
20	ATOM 5045 N ILE A 17	-18.521	12.393	34.614	1.00	12.65	A N
	ATOM 5046 CA ILE A 17	-18.549	13.621	33.823	1.00	12.45	A C
	ATOM 5047 CB ILE A 17	-17.659	13.507	32.548	1.00	11.09	A C
	ATOM 5048 CG2 ILE A 17	-18.158	12.384	31.642	1.00	9.92	A C
	ATOM 5049 CG1 ILE A 17	-17.663	14.836	31.790	1.00	11.02	A C
25	ATOM 5050 CD1 ILE A 17	-17.127	16.025	32.594	1.00	13.12	A C

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	ATOM 5051 C	ILE A	17	-19.981	13.984	33.430	1.00	12.64	A C
	ATOM 5052 O	ILE A	17	-20.348	15.155	33.421	1.00	13.53	A O
	ATOM 5242 N	TRP A	39	-24.802	-7.318	35.073	1.00	35.03	A N
	ATOM 5243 CA	TRP A	39	-24.074	-6.905	33.874	1.00	33.95	A C
5	ATOM 5244 CB	TRP A	39	-22.586	-6.705	34.193	1.00	30.71	A C
	ATOM 5245 G	TRP A	39	-21.787	-6.208	33.021	1.00	27.71	A C
	ATOM 5246 CD2	TRP A	39	-22.182	-5.206	32.072	1.00	26.24	A C
	ATOM 5247 CE2	TRP A	39	-21.134	-5.085	31.130	1.00	27.24	A C
	ATOM 5248 CE3	TRP A	39	-23.319	-4.401	31.925	1.00	25.00	A C
10	ATOM 5249 CD1	TRP A	39	-20.549	-6.637	32.630	1.00	28.16	A C
	ATOM 5250 NE1	TRP A	39	-20.152	-5.969	31.493	1.00	28.63	A N
	ATOM 5251 CZ2	TRP A	39	-21.191	-4.191	30.054	1.00	26.14	A C
	ATOM 5252 CZ3	TRP A	39	-23.377	-3.511	30.850	1.00	24.88	A C
	ATOM 5253 CH2	TRP A	39	-22.318	-3.416	29.931	1.00	25.30	A C
15	ATOM 5254 C	TRP A	39	-24.217	-7.861	32.683	1.00	34.33	A C
	ATOM 5255 O	TRP A	39	-24.633	-7.451	31.600	1.00	34.30	A O
	ATOM 5256 N	PRO A	40	-23.880	-9.149	32.869	1.00	35.19	A N
	ATOM 5257 CD	PRO A	40	-23.513	-9.824	34.128	1.00	35.28	A C
	ATOM 5258 CA	PRO A	40	-23.985	-10.120	31.775	1.00	35.54	A C
20	ATOM 5259 CB	PRO A	40	-23.906	-11.460	32.499	1.00	36.12	A C
	ATOM 5260 CG	PRO A	40	-22.984	-11.156	33.638	1.00	36.50	A C
	ATOM 5261 C	PRO A	40	-25.259	-9.985	30.946	1.00	35.56	A C
	ATOM 5262 O	PRO A	40	-25.200	-9.824	29.727	1.00	36.61	A O
	ATOM 5263 N	GLU A	41	-26.406	-10.043	31.614	1.00	34.82	A N
25	ATOM 5264 CA	GLU A	41	-27.693	-9.942	30.935	1.00	35.20	A C

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	ATOM 5265 CB	GLU A	41	-28.833	-10.189	31.931	1.00	37.14	A C
	ATOM 5266 CG	GLU A	41	-30.221	-10.044	31.328	1.00	41.54	A C
	ATOM 5267 CD	GLU A	41	-30.489	-11.046	30.219	1.00	44.14	A C
	ATOM 5268 OE1	GLU A	41	-31.529	-10.915	29.536	1.00	46.32	A O
5	ATOM 5269 OE2	GLU A	41	-29.665	-11.967	30.030	1.00	45.36	A O
	ATOM 5270 C	GLU A	41	-27.911	-8.603	30.237	1.00	33.75	A C
	ATOM 5271 O	GLU A	41	-28.460	-8.553	29.135	1.00	34.40	A O
	ATOM 5272 N	ILE A	42	-27.483	-7.521	30.880	1.00	31.53	A N
	ATOM 5273 CA	ILE A	42	-27.648	-6.181	30.322	1.00	28.99	A C
10	ATOM 5274 CB	ILE A	42	-27.401	-5.106	31.402	1.00	28.48	A C
	ATOM 5275 CG2	ILE A	42	-27.689	-3.721	30.833	1.00	27.91	A C
	ATOM 5276 CG1	ILE A	42	-28.304	-5.369	32.608	1.00	27.61	A C
	ATOM 5277 CD1	ILE A	42	-27.975	-4.530	33.821	1.00	29.35	A C
	ATOM 5278 C	ILE A	42	-26.709	-5.926	29.143	1.00	27.64	A C
15	ATOM 5279 O	ILE A	42	-27.114	-5.355	28.129	1.00	27.10	A O
	ATOM 5280 N	LYS A	43	-25.459	-6.353	29.283	1.00	26.84	A N
	ATOM 5281 CA	LYS A	43	-24.457	-6.173	28.237	1.00	27.71	A C
	ATOM 5282 CB	LYS A	43	-23.160	-6.886	28.629	1.00	26.22	A C
	ATOM 5283 CG	LYS A	43	-22.062	-6.814	27.579	1.00	23.72	A C
20	ATOM 5284 CD	LYS A	43	-20.871	-7.669	27.981	1.00	22.67	A C
	ATOM 5285 CE	LYS A	43	-19.747	-7.576	26.965	1.00	23.33	A C
	ATOM 5286 NZ	LYS A	43	-19.134	-6.217	26.936	1.00	21.56	A N
	ATOM 5287 C	LYS A	43	-24.940	-6.708	26.893	1.00	28.75	A C
	ATOM 5288 O	LYS A	43	-24.719	-6.090	25.852	1.00	28.75	A O
25	ATOM 5328 N	GLY A	49	-22.268	-3.248	23.763	1.00	15.23	A N

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	ATOM 5329	CA	GLY A	49	-21.927	-3.903	25.015	1.00	15.04	A C
	ATOM 5330	C	GLY A	49	-21.064	-3.144	26.005	1.00	15.33	A C
	ATOM 5331	O	GLY A	49	-20.313	-3.754	26.768	1.00	15.11	A O
	ATOM 5332	N	LYS A	50	-21.169	-1.821	26.007	1.00	13.57	A N
5	ATOM 5333	CA	LYS A	50	-20.380	-1.008	26.926	1.00	14.57	A C
	ATOM 5334	CB	LYS A	50	-19.259	-0.274	26.173	1.00	15.57	A C
	ATOM 5335	CG	LYS A	50	-18.310	-1.166	25.391	1.00	18.60	A C
	ATOM 5336	CD	LYS A	50	-17.505	-2.069	26.308	1.00	21.95	A C
	ATOM 5337	CE	LYS A	50	-16.603	-2.992	25.504	1.00	24.43	A C
10	ATOM 5338	NZ	LYS A	50	-15.681	-2.218	24.631	1.00	25.99	A N
	ATOM 5339	C	LYS A	50	-21.246	0.030	27.625	1.00	14.42	A C
	ATOM 5340	O	LYS A	50	-22.253	0.488	27.081	1.00	14.19	A O
	ATOM 5341	N	ILE A	51	-20.848	0.394	28.840	1.00	14.37	A N
	ATOM 5342	CA	ILE A	51	-21.553	1.416	29.597	1.00	14.74	A C
15	ATOM 5343	CB	ILE A	51	-22.203	0.840	30.876	1.00	15.30	A C
	ATOM 5344	CG2	ILE A	51	-23.403	-0.008	30.497	1.00	17.79	A C
	ATOM 5345	CG1	ILE A	51	-21.187	0.020	31.675	1.00	15.08	A C
	ATOM 5346	CD1	ILE A	51	-21.764	-0.585	32.950	1.00	15.84	A C
	ATOM 5347	C	ILE A	51	-20.526	2.490	29.949	1.00	14.66	A C
20	ATOM 5348	O	ILE A	51	-19.324	2.232	29.931	1.00	16.06	A O
	ATOM 5349	N	PRO A	52	-20.982	3.700	30.299	1.00	15.26	A N
	ATOM 5350	CD	PRO A	52	-20.083	4.841	30.562	1.00	16.04	A C
	ATOM 5351	CA	PRO A	52	-22.379	4.124	30.396	1.00	15.40	A C
	ATOM 5352	CB	PRO A	52	-22.276	5.409	31.197	1.00	15.83	A C
25	ATOM 5353	CG	PRO A	52	-21.045	6.024	30.593	1.00	15.77	A C

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	ATOM 5354 C	PRO A	52	-23.101	4.365	29.080	1.00	16.83	A C
	ATOM 5355 O	PRO A	52	-22.492	4.484	28.015	1.00	14.90	A O
	ATOM 5356 N	ILE A	53	-24.420	4.438	29.188	1.00	17.77	A N
	ATOM 5357 CA	ILE A	53	-25.288	4.730	28.067	1.00	18.90	A C
5	ATOM 5358 CB	ILE A	53	-26.045	3.483	27.563	1.00	20.61	A C
	ATOM 5359 CG2	ILE A	53	-25.054	2.435	27.075	1.00	20.84	A C
	ATOM 5360 CG1	ILE A	53	-26.938	2.928	28.675	1.00	21.82	A C
	ATOM 5361 CD1	ILE A	53	-27.891	1.842	28.211	1.00	24.03	A C
	ATOM 5362 C	ILE A	53	-26.286	5.708	28.662	1.00	18.88	A C
10	ATOM 5363 O	ILE A	53	-26.494	5.722	29.878	1.00	18.43	A O
	ATOM 5423 N	HIS A	62	-24.373	6.192	23.498	1.00	15.70	A N
	ATOM 5424 CA	HIS A	62	-23.236	5.561	24.160	1.00	15.77	A C
	ATOM 5425 CB	HIS A	62	-22.957	4.167	23.568	1.00	15.57	A C
	ATOM 5426 CG	HIS A	62	-22.517	4.179	22.134	1.00	14.35	A C
15	ATOM 5427 CD2	HIS A	62	-21.358	3.778	21.556	1.00	15.17	A C
	ATOM 5428 ND1	HIS A	62	-23.332	4.598	21.104	1.00	17.10	A N
	ATOM 5429 CE1	HIS A	62	-22.697	4.451	19.953	1.00	14.96	A C
	ATOM 5430 NE2	HIS A	62	-21.498	3.955	20.200	1.00	15.48	A N
	ATOM 5431 C	HIS A	62	-21.988	6.437	24.080	1.00	14.50	A C
20	ATOM 5432 O	HIS A	62	-22.007	7.489	23.442	1.00	13.29	A O
	ATOM 5433 N	GLN A	63	-20.913	5.997	24.734	1.00	13.87	A N
	ATOM 5434 CA	GLN A	63	-19.654	6.740	24.764	1.00	12.90	A C
	ATOM 5435 CB	GLN A	63	-19.224	7.137	23.345	1.00	12.53	A C
	ATOM 5436 CG	GLN A	63	-18.581	6.001	22.545	1.00	11.52	A C
25	ATOM 5437 CD	GLN A	63	-17.268	5.533	23.160	1.00	12.20	A C

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	ATOM 5438	OE1	GLN	A	63	-16.730	6.176	24.062	1.00	10.43	A	O
	ATOM 5439	NE2	GLN	A	63	-16.741	4.421	22.664	1.00	9.56	A	N
	ATOM 5440	C	GLN	A	63	-19.805	7.976	25.653	1.00	13.56	A	C
	ATOM 5441	O	GLN	A	63	-20.476	8.947	25.289	1.00	14.92	A	O
5	ATOM 5442	N	SER	A	64	-19.167	7.924	26.817	1.00	10.97	A	N
	ATOM 5443	CA	SER	A	64	-19.236	8.993	27.807	1.00	10.05	A	C
	ATOM 5444	CB	SER	A	64	-18.322	8.658	28.995	1.00	9.89	A	C
	ATOM 5445	OG	SER	A	64	-16.955	8.727	28.627	1.00	8.82	A	O
	ATOM 5446	C	SER	A	64	-18.932	10.411	27.323	1.00	8.80	A	C
10	ATOM 5447	O	SER	A	64	-19.674	11.339	27.636	1.00	9.79	A	O
	ATOM 5448	N	LEU	A	65	-17.853	10.586	26.565	1.00	8.85	A	N
	ATOM 5449	CA	LEU	A	65	-17.483	11.917	26.091	1.00	8.19	A	C
	ATOM 5450	CB	LEU	A	65	-16.009	11.933	25.671	1.00	7.83	A	C
	ATOM 5451	CG	LEU	A	65	-15.054	11.409	26.757	1.00	11.60	A	C
15	ATOM 5452CD1	LEU	A	65	-13.618	11.479	26.253	1.00	11.43	A	C	
	ATOM 5453	CD2	LEU	A	65	-15.220	12.226	28.041	1.00	8.48	A	C
	ATOM 5454	C	LEU	A	65	-18.374	12.419	24.956	1.00	10.81	A	C
	ATOM 5455	O	LEU	A	65	-18.539	13.627	24.779	1.00	11.65	A	O
	ATOM 5662	N	ASP	A	93	-9.664	14.664	25.566	1.00	7.26	A	N
20	ATOM 5663	CA	ASP	A	93	-9.071	13.449	25.009	1.00	6.80	A	C
	ATOM 5664	CB	ASP	A	93	-9.016	13.526	23.476	1.00	7.94	A	C
	ATOM 5665	CG	ASP	A	93	-10.318	13.092	22.823	1.00	9.46	A	C
	ATOM 5666	OD1	ASP	A	93	-10.361	12.988	21.577	1.00	10.43	A	O
	ATOM 5667	OD2	ASP	A	93	-11.302	12.855	23.556	1.00	6.66	A	O
25	ATOM 5668	C	ASP	A	93	-7.678	13.144	25.562	1.00	8.24	A	C

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	ATOM 5669 O	ASP A	93	-7.325	11.979	25.751	1.00	8.03	A O
	ATOM 5670 N	THR A	94	-6.879	14.179	25.808	1.00	7.87	A N
	ATOM 5671 CA	THR A	94	-5.541	13.973	26.354	1.00	7.89	A C
	ATOM 5672 CB	THR A	94	-4.753	15.305	26.444	1.00	8.49	A C
5	ATOM 5673 OG1	THR A	94	-4.329	15.693	25.125	1.00	8.47	A O
	ATOM 5674 CG2	THR A	94	-3.520	15.155	27.342	1.00	8.64	A C
	ATOM 5675 C	THR A	94	-5.679	13.342	27.740	1.00	8.60	A C
	ATOM 5676 O	THR A	94	-4.912	12.455	28.110	1.00	8.25	A O
	ATOM 5677 N	LEU A	95	-6.669	13.797	28.499	1.00	8.02	A N
10	ATOM 5678 CA	LEU A	95	-6.905	13.248	29.826	1.00	7.48	A C
	ATOM 5679 CB	LEU A	95	-7.884	14.135	30.606	1.00	6.39	A C
	ATOM 5680 CG	LEU A	95	-7.345	15.483	31.102	1.00	6.45	A C
	ATOM 5681 CD1	LEU A	95	-8.480	16.323	31.676	1.00	7.27	A C
	ATOM 5682 CD2	LEU A	95	-6.270	15.244	32.156	1.00	8.71	A C
15	ATOM 5683 C	LEU A	95	-7.464	11.829	29.700	1.00	8.84	A C
	ATOM 5684 O	LEU A	95	-7.013	10.921	30.394	1.00	6.72	A O
	ATOM 5685 N	ASP A	96	-8.426	11.639	28.794	1.00	9.13	A N
	ATOM 5686 CA	ASP A	96	-9.042	10.328	28.600	1.00	8.40	A C
	ATOM 5687 CB	ASP A	96	-10.213	10.421	27.614	1.00	9.89	A C
20	ATOM 5688 CG	ASP A	96	-11.200	9.271	27.768	1.00	8.95	A C
	ATOM 5689 OD1	ASP A	96	-11.674	9.046	28.903	1.00	11.48	A O
	ATOM 5690 OD2	ASP A	96	-11.515	8.599	26.761	1.00	8.48	A O
	ATOM 5691 C	ASP A	96	-8.029	9.294	28.113	1.00	11.25	A C
	ATOM 5692 O	ASP A	96	-8.083	8.129	28.516	1.00	11.68	A O
25	ATOM 5693 N	ASP A	97	-7.107	9.714	27.249	1.00	10.40	A N

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	ATOM 5694	CA	ASP	A	97	-6.074	8.815	26.748	1.00	10.66	A	C
	ATOM 5695	CB	ASP	A	97	-5.108	9.552	25.815	1.00	9.42	A	C
	ATOM 5696	CG	ASP	A	97	-5.684	9.804	24.429	1.00	10.69	A	C
	ATOM 5697	OD1	ASP	A	97	-5.100	10.644	23.708	1.00	8.34	A	O
5	ATOM 5698	OD2	ASP	A	97	-6.693	9.166	24.050	1.00	9.39	A	O
	ATOM 5699	C	ASP	A	97	-5.266	8.241	27.914	1.00	10.28	A	C
	ATOM 5700	O	ASP	A	97	-5.013	7.039	27.972	1.00	9.67	A	O
	ATOM 5701	N	PHE	A	98	-4.856	9.106	28.839	1.00	11.06	A	N
	ATOM 5702	CA	PHE	A	98	-4.057	8.667	29.984	1.00	13.17	A	C
10	ATOM 5703	CB	PHE	A	98	-3.508	9.871	30.767	1.00	12.79	A	C
	ATOM 5704	CG	PHE	A	98	-2.540	9.487	31.861	1.00	14.46	A	C
	ATOM 5705	CD1	PHE	A	98	-1.365	8.800	31.558	1.00	14.40	A	C
	ATOM 5706	CD2	PHE	A	98	-2.817	9.781	33.191	1.00	15.98	A	C
	ATOM 5707	CE1	PHE	A	98	-0.480	8.409	32.568	1.00	17.26	A	C
15	ATOM 5708	CE2	PHE	A	98	-1.938	9.394	34.214	1.00	16.31	A	C
	ATOM 5709	CZ	PHE	A	98	-0.769	8.706	33.899	1.00	14.31	A	C
	ATOM 5710	C	PHE	A	98	-4.828	7.754	30.935	1.00	14.11	A	C
	ATOM 5711	O	PHE	A	98	-4.308	6.731	31.381	1.00	14.82	A	O
	ATOM 5712	N	MET	A	99	-6.063	8.125	31.252	1.00	14.73	A	N
20	ATOM 5713	CA	MET	A	99	-6.886	7.318	32.149	1.00	14.22	A	C
	ATOM 5714	CB	MET	A	99	-8.225	8.013	32.420	1.00	15.31	A	C
	ATOM 5715	CG	MET	A	99	-8.121	9.374	33.109	1.00	15.68	A	C
	ATOM 5716	SD	MET	A	99	-7.267	9.310	34.694	1.00	15.84	A	S
	ATOM 5717	CE	MET	A	99	-8.515	8.541	35.722	1.00	16.08	A	C
25	ATOM 5718	C	MET	A	99	-7.150	5.939	31.548	1.00	16.86	A	C

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	ATOM 5719 O	MET A 99	-7.220	4.939	32.267	1.00	14.67	A O
	ATOM 5720 N	SER A 100	-7.292	5.892	30.225	1.00	16.11	A N
	ATOM 5721 CA	SER A 100	-7.561	4.641	29.523	1.00	16.96	A C
	ATOM 5722 CB	SER A 100	-8.084	4.936	28.115	1.00	16.86	A C
5	ATOM 5723 OG	SER A 100	-9.356	5.556	28.184	1.00	16.40	A O
	ATOM 5724 C	SER A 100	-6.350	3.717	29.442	1.00	19.01	A C
	ATOM 5725 O	SER A 100	-6.489	2.528	29.149	1.00	19.47	A O
	ATOM 5726 N	CYS A 101	-5.166	4.262	29.697	1.00	20.58	A N
	ATOM 5727 CA	CYS A 101	-3.944	3.464	29.665	1.00	23.67	A C
10	ATOM 5728 CB	CYS A 101	-2.707	4.368	29.693	1.00	26.07	A C
	ATOM 5729 SG	CYS A 101	-2.263	5.097	28.099	1.00	30.40	A S
	ATOM 5730 C	CYS A 101	-3.876	2.484	30.836	1.00	23.47	A C
	ATOM 5731 O	CYS A 101	-3.257	1.426	30.729	1.00	24.00	A O
	ATOM 5732 N	PHE A 102	-4.504	2.833	31.953	1.00	23.47	A N
15	ATOM 5733 CA	PHE A 102	-4.485	1.955	33.117	1.00	24.57	A C
	ATOM 5734 CB	PHE A 102	-5.012	2.681	34.360	1.00	22.30	A C
	ATOM 5735 CG	PHE A 102	-4.128	3.798	34.832	1.00	21.46	A C
	ATOM 5736 CD1	PHE A 102	-4.099	5.014	34.158	1.00	20.64	A C
	ATOM 5737 CD2	PHE A 102	-3.313	3.631	35.949	1.00	20.02	A C
20	ATOM 5738 CE1	PHE A 102	-3.267	6.055	34.590	1.00	21.12	A C
	ATOM 5739 CE2	PHE A 102	-2.480	4.662	36.387	1.00	20.36	A C
	ATOM 5740 CZ	PHE A 102	-2.458	5.875	35.705	1.00	18.32	A C
	ATOM 5741 C	PHE A 102	-5.313	0.698	32.881	1.00	25.48	A C
	ATOM 5742 O	PHE A 102	-6.423	0.765	32.358	1.00	25.08	A O
25	ATOM 5743 N	PRO A 103	-4.773	-0.471	33.259	1.00	27.90	A N

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	ATOM 5744 CD	PRO A 103	-3.398	-0.682	33.750	1.00	27.31	A C
	ATOM 5745 CA	PRO A 103	-5.466	-1.751	33.090	1.00	29.68	A C
	ATOM 5746 CB	PRO A 103	-4.323	-2.753	33.124	1.00	28.70	A C
	ATOM 5747 CG	PRO A 103	-3.410	-2.145	34.142	1.00	28.84	A C
5	ATOM 5748 C	PRO A 103	-6.471	-1.975	34.220	1.00	31.64	A C
	ATOM 5749 O	PRO A 103	-6.208	-2.740	35.150	1.00	32.46	A O
	ATOM 5750 N	TRP A 104	-7.619	-1.308	34.132	1.00	33.14	A N
	ATOM 5751 CA	TRP A 104	-8.652	-1.416	35.157	1.00	34.92	A C
	ATOM 5752 CB	TRP A 104	-9.740	-0.360	34.936	1.00	34.59	A C
10	ATOM 5753 CG	TRP A 104	-9.223	1.041	34.784	1.00	33.67	A C
	ATOM 5754 CD2	TRP A 104	-8.909	1.959	35.838	1.00	32.46	A C
	ATOM 5755 CE2	TRP A 104	-8.451	3.149	35.233	1.00	33.36	A C
	ATOM 5756 CE3	TRP A 104	-8.970	1.891	37.237	1.00	32.51	A C
	ATOM 5757 CD1	TRP A 104	-8.949	1.692	33.615	1.00	33.31	A C
15	ATOM 5758 NE1	TRP A 104	-8.486	2.960	33.876	1.00	33.69	A N
	ATOM 5759 CZ2	TRP A 104	-8.057	4.265	35.980	1.00	33.19	A C
	ATOM 5760 CZ3	TRP A 104	-8.577	3.002	37.979	1.00	31.26	A C
	ATOM 5761 CH2	TRP A 104	-8.127	4.171	37.347	1.00	32.36	A C
	ATOM 5762 C	TRP A 104	-9.314	-2.787	35.225	1.00	36.55	A C
20	ATOM 5763 O	TRP A 104	-9.542	-3.317	36.312	1.00	36.03	A O
	ATOM 5764 N	ALA A 105	-9.629	-3.353	34.064	1.00	39.05	A N
	ATOM 5765 CA	ALA A 105	-10.285	-4.657	34.001	1.00	41.04	A C
	ATOM 5766 CB	ALA A 105	-11.224	-4.709	32.801	1.00	41.47	A C
	ATOM 5767 C	ALA A 105	-9.293	-5.812	33.936	1.00	42.49	A C
25	ATOM 5768 O	ALA A 105	-9.615	-6.891	33.436	1.00	43.00	A O

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	ATOM 5769 N	GLU A 106	-8.087	-5.583	34.443	1.00	43.51	A N
	ATOM 5770 CA	GLU A 106	-7.055	-6.610	34.442	1.00	44.47	A C
	ATOM 5771 CB	GLU A 106	-5.669	-5.960	34.381	1.00	44.70	A C
	ATOM 5772 CG	GLU A 106	-4.502	-6.940	34.373	1.00	45.21	A C
5	ATOM 5773 CD	GLU A 106	-4.626	-7.993	33.289	1.00	46.80	A C
	ATOM 5774 OE1	GLU A 106	-5.375	-8.974	33.490	1.00	47.31	A O
	ATOM 5775 OE2	GLU A 106	-3.982	-7.837	32.230	1.00	46.33	A O
	ATOM 5776	GLU A 106	-7.170	-7.483	35.688	1.00	44.69	A C
	ATOM 5777 O	GLU A 106	-7.174	-6.980	36.812	1.00	43.85	A
10	O							
	ATOM 5778 N	LYS A 107	-7.275	-8.791	35.477	1.00	46.22	A N
	ATOM 5779 CA	LYS A 107	-7.386	-9.744	36.576	1.00	47.90	A C
	ATOM 5780 CB	LYS A 107	-8.160	-10.985	36.124	1.00	48.02	A C
	ATOM 5781 CG	LYS A 107	-9.649	-10.743	35.925	1.00	48.88	A C
15	ATOM 5782 CD	LYS A 107	-10.315	-10.333	37.233	1.00	49.71	A C
	ATOM 5783 CE	LYS A 107	-11.799	-10.060	37.043	1.00	50.86	A C
	ATOM 5784 NZ	LYS A 107	-12.534	-11.251	36.534	1.00	51.17	A N
	ATOM 5785 C	LYS A 107	-6.010	-10.148	37.096	1.00	48.88	A C
	ATOM 5786 O	LYS A 107	-5.847	-10.426	38.284	1.00	49.63	A O
20	ATOM 5787 N	LYS A 108	-5.025	-10.179	36.204	1.00	49.39	A N
	ATOM 5788 CA	LYS A 108	-3.662	-10.534	36.584	1.00	50.95	A C
	ATOM 5789 CB	LYS A 108	-2.780	-10.649	35.338	1.00	50.92	A C
	ATOM 5790 CG	LYS A 108	-3.244	-11.706	34.349	1.00	51.30	A C
	ATOM 5791 CD	LYS A 108	-2.370	-11.744	33.100	1.00	51.21	A C
25	ATOM 5792 CE	LYS A 108	-2.474	-10.450	32.306	1.00	51.88	A C

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	ATOM 5793 NZ	LYS A 108	-1.733	-10.517	31.015	1.00	51.47	A N
	ATOM 5794 C	LYS A 108	-3.115	-9.452	37.514	1.00	51.93	A C
	ATOM 5795 O	LYS A 108	-2.605	-8.428	37.057	1.00	52.21	A O
	ATOM 5796 N	GLN A 109	-3.228	-9.687	38.818	1.00	53.19	A N
5	ATOM 5797 CA	GLN A 109	-2.770	-8.734	39.827	1.00	54.34	A C
	ATOM 5798 CB	GLN A 109	-3.029	-9.293	41.229	1.00	55.53	A C
	ATOM 5799 CG	GLN A 109	-2.808	-8.292	42.359	1.00	57.97	A C
	ATOM 5800 CD	GLN A 109	-3.896	-7.230	42.433	1.00	59.38	A C
	ATOM 5801 OE1	GLN A 109	-3.833	-6.318	43.260	1.00	60.01	A O
10	ATOM 5802 NE2	GLN A 109	-4.903	-7.349	41.572	1.00	59.24	A
	N							
	ATOM 5803 C	GLN A 109	-1.291	-8.372	39.689	1.00	53.97	A C
	ATOM 5804 O	GLN A 109	-0.900	-7.231	39.939	1.00	54.03	A O
	ATOM 5805 N	ASP A 110	-0.473	-9.344	39.296	1.00	53.79	A N
15	ATOM 5806 CA	ASP A 110	0.961	-9.120	39.136	1.00	53.28	A C
	ATOM 5807 CB	ASP A 110	1.687	-10.460	38.967	1.00	54.50	A C
	ATOM 5808 CG	ASP A 110	1.180	-11.256	37.777	1.00	56.41	A C
	ATOM 5809 OD1	ASP A 110	-0.040	-11.516	37.708	1.00	57.39	A O
	ATOM 5810 OD2	ASP A 110	2.005	-11.626	36.913	1.00	57.49	A O
20	ATOM 5811 C	ASP A 110	1.276	-8.203	37.956	1.00	52.12	A C
	ATOM 5812 O	ASP A 110	2.309	-7.532	37.939	1.00	52.35	A O
	ATOM 5813 N	VAL A 111	0.381	-8.173	36.975	1.00	50.53	A N
	ATOM 5814 CA	VAL A 111	0.565	-7.340	35.792	1.00	48.09	A C
	ATOM 5815 CB	VAL A 111	-0.020	-8.032	34.541	1.00	47.90	A C
25	ATOM 5816 CG1	VAL A 111	0.175	-7.153	33.313	1.00	47.07	A C

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	ATOM 5817	CG2	VAL A	111	0.649	-9.382	34.343	1.00	46.18	A C
	ATOM 5818	C	VAL A	111	-0.106	-5.980	35.973	1.00	47.23	A C
	ATOM 5819	O	VAL A	111	0.392	-4.959	35.497	1.00	46.02	A O
	ATOM 5820	N	LYS A	112	-1.237	-5.974	36.670	1.00	46.23	A N
5	ATOM 5821	CA	LYS A	112	-1.981	-4.746	36.918	1.00	45.70	A C
	ATOM 5822	CB	LYS A	112	-3.328	-5.076	37.563	1.00	45.91	A C
	ATOM 5823	CG	LYS A	112	-4.205	-3.866	37.828	1.00	47.00	A C
	ATOM 5824	CD	LYS A	112	-5.587	-4.288	38.294	1.00	46.65	A C
	ATOM 5825	CE	LYS A	112	-6.505	-3.093	38.472	1.00	47.06	A C
10	ATOM 5826	NZ	LYS A	112	-7.882	-3.530	38.822	1.00	47.01	A N
	ATOM 5827	C	LYS A	112	-1.197	-3.793	37.815	1.00	45.36	A C
	ATOM 5828	O	LYS A	112	-1.044	-2.611	37.499	1.00	43.76	A O
	ATOM 5829	N	GLU A	113	-0.700	-4.316	38.931	1.00	45.30	A N
	ATOM 5830	CA	GLU A	113	0.065	-3.520	39.885	1.00	45.81	A C
15	ATOM 5831	CB	GLU A	113	0.434	-4.377	41.100	1.00	46.58	A C
	ATOM 5832	CG	GLU A	113	0.985	-3.602	42.292	1.00	46.95	A C
	ATOM 5833	CD	GLU A	113	-0.079	-2.797	43.024	1.00	47.25	A C
	ATOM 5834	OE1	GLU A	113	0.232	-2.252	44.104	1.00	47.79	A O
	ATOM 5835	OE2	GLU A	113	-1.222	-2.708	42.526	1.00	46.47	A O
20	ATOM 5836	C	GLU A	113	1.335	-2.963	39.244	1.00	45.70	A C
	ATOM 5837	O	GLU A	113	1.734	-1.832	39.520	1.00	45.29	A O
	ATOM 5838	N	GLN A	114	1.961	-3.764	38.386	1.00	45.03	A N
	ATOM 5839	CA	GLN A	114	3.188	-3.364	37.703	1.00	44.59	A C
	ATOM 5840	CB	GLN A	114	3.757	-4.554	36.919	1.00	46.95	A C
25	ATOM 5841	CG	GLN A	114	5.090	-4.301	36.224	1.00	49.65	A C

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	ATOM 5842	CD	GLN A 114	4.949	-3.515	34.933	1.00	51.80	A C
	ATOM 5843	OE1	GLN A 114	4.223	-3.920	34.024	1.00	54.22	A O
	ATOM 5844	NE2	GLN A 114	5.650	-2.389	34.842	1.00	52.38	A N
	ATOM 5845	C	GLN A 114	2.956	-2.179	36.767	1.00	43.31	A C
5	ATOM 5846	O	GLN A 114	3.720	-1.214	36.778	1.00	43.59	A O
	ATOM 5847	N	MET A 115	1.902	-2.252	35.960	1.00	40.98	A N
	ATOM 5848	CA	MET A 115	1.586	-1.175	35.026	1.00	38.92	A C
	ATOM 5849	CB	MET A 115	0.543	-1.646	34.006	1.00	40.82	A C
	ATOM 5850	CG	MET A 115	0.066	-0.553	33.052	1.00	43.23	A C
10	ATOM 5851	SD	MET A 115	1.400	0.229	32.107	1.00	46.86	A S
	ATOM 5852	CE	MET A 115	0.903	-0.150	30.414	1.00	46.99	A C
	ATOM 5853	C	MET A 115	1.080	0.073	35.750	1.00	36.12	A C
	ATOM 5854	O	MET A 115	1.414	1.195	35.366	1.00	34.59	A O
	ATOM 5855	N	PHE A 116	0.277	-0.124	36.793	1.00	33.79	A N
15	ATOM 5856	CA	PHE A 116	-0.260	0.997	37.563	1.00	31.55	A C
	ATOM 5857	CB	PHE A 116	-1.101	0.496	38.740	1.00	29.74	A C
	ATOM 5858	CG	PHE A 116	-2.580	0.648	38.544	1.00	26.92	A C
	ATOM 5859	CD1	PHE A 116	-3.277	-0.205	37.697	1.00	26.13	A C
	ATOM 5860	CD2	PHE A 116	-3.280	1.647	39.214	1.00	25.49	A C
20	ATOM 5861	CE1	PHE A 116	-4.652	-0.069	37.520	1.00	25.62	A C
	ATOM 5862	CE2	PHE A 116	-4.655	1.795	39.045	1.00	24.62	A C
	ATOM 5863	CZ	PHE A 116	-5.343	0.935	38.196	1.00	25.52	A C
	ATOM 5864	C	PHE A 116	0.852	1.885	38.108	1.00	31.56	A C
	ATOM 5865	O	PHE A 116	0.850	3.100	37.905	1.00	29.53	A O
25	ATOM 6152	N	TYR A 152	-13.728	17.655	33.722	1.00	8.61	A N

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	ATOM 6153 CA TYR A 152	-13.021	16.402	33.504	1.00	9.79	A C
	ATOM 6154 CB TYR A 152	-12.841	16.120	32.003	1.00	7.44	A C
	ATOM 6155 CG TYR A 152	-12.799	14.634	31.704	1.00	8.27	A C
	ATOM 6156 CD1 TYR A 152	-13.773	13.778	32.225	1.00	8.38	A C
5	ATOM 6157 CE1 TYR A 152	-13.742	12.403	31.973	1.00	10.32	A C
	ATOM 6158 CD2 TYR A 152	-11.791	14.080	30.919	1.00	5.95	A C
	ATOM 6159 CE2 TYR A 152	-11.751	12.704	30.659	1.00	8.41	A C
	ATOM 6160 CZ TYR A 152	-12.729	11.873	31.191	1.00	8.47	A C
	ATOM 6161 OH TYR A 152	-12.695	10.517	30.951	1.00	9.30	A O
10	ATOM 6162 C TYR A 152	-11.671	16.387	34.209	1.00	10.81	A C
	ATOM 6163 O TYR A 152	-11.237	15.344	34.695	1.00	13.37	A O
	ATOM 6164 N TRP A 153	-11.002	17.536	34.274	1.00	11.77	A N
	ATOM 6165 CA TRP A 153	-9.715	17.589	34.964	1.00	12.66	A C
	ATOM 6166 CB TRP A 153	-9.082	18.981	34.855	1.00	13.54	A C
15	ATOM 6167 CG TRP A 153	-8.073	19.251	35.950	1.00	13.64	A C
	ATOM 6168 CD2 TRP A 153	-6.880	18.503	36.230	1.00	12.79	A C
	ATOM 6169 CE2 TRP A 153	-6.280	19.084	37.372	1.00	13.87	A C
	ATOM 6170 CE3 TRP A 153	-6.260	17.400	35.629	1.00	14.97	A C
	ATOM 6171 CD1 TRP A 153	-8.143	20.228	36.906	1.00	14.04	A C
20	ATOM 6172 NE1 TRP A 153	-7.071	20.132	37.763	1.00	14.10	A N
	ATOM 6173 CZ2 TRP A 153	-5.088	18.596	37.927	1.00	12.50	A C
	ATOM 6174 CZ3 TRP A 153	-5.072	16.914	36.183	1.00	14.36	A C
	ATOM 6175 CH2 TRP A 153	-4.502	17.516	37.321	1.00	14.19	A C
	ATOM 6176 C TRP A 153	-9.878	17.232	36.441	1.00	11.85	A C
25	ATOM 6177 O TRP A 153	-9.107	16.434	36.981	1.00	12.51	A O

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	ATOM 6178 N	GLU A 154	-10.883	17.817	37.089	1.00	11.73	A N
	ATOM 6179 CA	GLU A 154	-11.134	17.564	38.512	1.00	10.94	A C
	ATOM 6180 CB	GLU A 154	-12.231	18.510	39.027	1.00	11.59	A C
	ATOM 6181 CG	GLU A 154	-12.404	18.521	40.546	1.00	11.01	A C
5	ATOM 6182 CD	GLU A 154	-13.332	17.431	41.059	1.00	16.21	A C
	ATOM 6183 OE1	GLU A 154	-13.328	17.170	42.284	1.00	14.24	A O
	ATOM 6184 OE2	GLU A 154	-14.078	16.842	40.248	1.00	16.08	A O
	ATOM 6185 C	GLU A 154	-11.536	16.108	38.739	1.00	11.33	A C
	ATOM 6186 O	GLU A 154	-11.134	15.477	39.725	1.00	11.71	A O
10	ATOM 6187 N	ILE A 155	-12.327	15.580	37.815	1.00	10.60	A N
	ATOM 6188 CA	ILE A 155	-12.790	14.200	37.880	1.00	10.68	A C
	ATOM 6189 CB	ILE A 155	-13.847	13.951	36.774	1.00	10.77	A C
	ATOM 6190 CG2	ILE A 155	-14.071	12.459	36.564	1.00	11.39	A C
	ATOM 6191 CG1	ILE A 155	-15.148	14.671	37.154	1.00	12.20	A C
15	ATOM 6192 CD1	ILE A 155	-16.192	14.711	36.048	1.00	9.68	A C
	ATOM 6193 C	ILE A 155	-11.630	13.210	37.750	1.00	11.46	A C
	ATOM 6194 O	ILE A 155	-11.493	12.292	38.567	1.00	12.61	A O
	ATOM 6195 N	CYS A 156	-10.789	13.402	36.735	1.00	10.83	A N
	ATOM 6196 CA	CYS A 156	-9.642	12.524	36.514	1.00	10.78	A C
20	ATOM 6197 CB	CYS A 156	-8.964	12.856	35.179	1.00	12.57	A C
	ATOM 6198 SG	CYS A 156	-9.924	12.424	33.698	1.00	11.44	A S
	ATOM 6199 C	CYS A 156	-8.610	12.617	37.642	1.00	11.39	A C
	ATOM 6200 O	CYS A 156	-8.078	11.600	38.090	1.00	10.94	A O
	ATOM 6201 N	SER A 157	-8.327	13.836	38.096	1.00	10.71	A N
25	ATOM 6202 CA	SER A 157	-7.348	14.035	39.160	1.00	11.64	A C

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	ATOM 6203 CB	SER A 157	-7.005	15.526	39.312	1.00	8.14	A C
	ATOM 6204 OG	SER A 157	-8.149	16.309	39.581	1.00	8.71	A O
	ATOM 6205 C	SER A 157	-7.815	13.463	40.493	1.00	11.79	A C
	ATOM 6206 O	SER A 157	-7.000	12.976	41.280	1.00	12.03	A O
5	ATOM 6207 N	THR A 158	-9.119	13.521	40.750	1.00	10.51	A N
	ATOM 6208 CA	THR A 158	-9.650	12.979	41.996	1.00	12.25	A C
	ATOM 6209 CB	THR A 158	-11.188	13.142	42.086	1.00	12.13	A C
	ATOM 6210 OG1	THR A 158	-11.512	14.507	42.379	1.00	11.92	A O
	ATOM 6211 CG2	THR A 158	-11.758	12.251	43.180	1.00	12.89	A C
10	ATOM 6212 C	THR A 158	-9.303	11.497	42.089	1.00	12.30	A C
	ATOM 6213 O	THR A 158	-8.873	11.015	43.135	1.00	13.28	A O
	ATOM 6214 N	THR A 159	-9.484	10.778	40.986	1.00	11.79	A N
	ATOM 6215 CA	THR A 159	-9.189	9.352	40.949	1.00	12.60	A C
	ATOM 6216 CB	THR A 159	-9.777	8.713	39.671	1.00	12.94	A C
15	ATOM 6217 OG1	THR A 159	-11.207	8.818	39.711	1.00	13.88	A O
	ATOM 6218 CG2	THR A 159	-9.383	7.243	39.570	1.00	13.31	A C
	ATOM 6219 C	THR A 159	-7.683	9.073	41.028	1.00	12.97	A C
	ATOM 6220 O	THR A 159	-7.242	8.210	41.792	1.00	13.33	A O
	ATOM 6221 N	LEU A 160	-6.891	9.801	40.247	1.00	11.91	A N
20	ATOM 6222 CA	LEU A 160	-5.449	9.602	40.272	1.00	11.99	A C
	ATOM 6223 CB	LEU A 160	-4.767	10.506	39.243	1.00	11.62	A C
	ATOM 6224 CG	LEU A 160	-5.052	10.201	37.764	1.00	10.47	A C
	ATOM 6225 CD1	LEU A 160	-4.377	11.244	36.896	1.00	11.07	A C
	ATOM 6226 CD2	LEU A 160	-4.547	8.806	37.399	1.00	9.49	A C
25	ATOM 6227 C	LEU A 160	-4.869	9.862	41.667	1.00	13.79	A C

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	ATOM 6228 O	LEU A 160	-3.954	9.157	42.101	1.00	12.53	A O
	ATOM 6229 N	LEU A 161	-5.408	10.863	42.364	1.00	13.03	A N
	ATOM 6230 CA	LEU A 161	-4.938	11.210	43.703	1.00	13.25	A C
	ATOM 6231 CB	LEU A 161	-5.638	12.476	44.209	1.00	13.43	A C
5	ATOM 6232 CG	LEU A 161	-5.137	13.820	43.672	1.00	14.45	A C
	ATOM 6233 CD1	LEU A 161	-6.127	14.924	44.045	1.00	11.48	A C
	ATOM 6234 CD2	LEU A 161	-3.751	14.118	44.237	1.00	13.53	A C
	ATOM 6235 C	LEU A 161	-5.145	10.080	44.704	1.00	15.09	A C
	ATOM 6236 O	LEU A 161	-4.415	9.979	45.691	1.00	16.09	A O
10	ATOM 6237 N	VAL A 162	-6.143	9.238	44.459	1.00	14.39	A N
	ATOM 6238 CA	VAL A 162	-6.411	8.116	45.344	1.00	14.43	A C
	ATOM 6239 CB	VAL A 162	-7.700	7.366	44.938	1.00	15.83	A C
	ATOM 6240 CG1	VAL A 162	-7.769	6.019	45.655	1.00	11.08	A C
	ATOM 6241 CG2	VAL A 162	-8.925	8.207	45.287	1.00	14.62	A C
15	ATOM 6242 C	VAL A 162	-5.242	7.140	45.304	1.00	15.52	A C
	ATOM 6243 O	VAL A 162	-4.861	6.579	46.329	1.00	16.41	A O
	ATOM 6244 N	PHE A 163	-4.667	6.951	44.119	1.00	14.68	A N
	ATOM 6245 CA	PHE A 163	-3.543	6.036	43.955	1.00	15.48	A C
	ATOM 6246 CB	PHE A 163	-3.660	5.286	42.624	1.00	16.17	A C
20	ATOM 6247 CG	PHE A 163	-4.915	4.476	42.498	1.00	17.77	A C
	ATOM 6248 CD1	PHE A 163	-6.066	5.026	41.934	1.00	18.11	A C
	ATOM 6249 CD2	PHE A 163	-4.962	3.172	42.978	1.00	17.18	A C
	ATOM 6250 CE1	PHE A 163	-7.243	4.284	41.852	1.00	18.08	A C
	ATOM 6251 CE2	PHE A 163	-6.134	2.422	42.901	1.00	17.00	A C
25	ATOM 6252 CZ	PHE A 163	-7.277	2.981	42.338	1.00	18.37	A C

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	ATOM 6253 C	PHE A 163	-2.179	6.714	44.041	1.00	15.57	A C
	ATOM 6254 O	PHE A 163	-1.164	6.044	44.214	1.00	16.24	A O
	ATOM 6528 N	THR A 197	-17.099	5.832	46.606	1.00	22.13	A N
	ATOM 6529 CA	THR A 197	-16.501	4.631	46.037	1.00	20.93	A C
5	ATOM 6530 CB	THR A 197	-17.228	4.228	44.740	1.00	20.53	A C
	ATOM 6531 OG1	THR A 197	-17.165	5.313	43.801	1.00	19.47	A O
	ATOM 6532 CG2	THR A 197	-18.687	3.904	45.031	1.00	19.28	A C
	ATOM 6533 C	THR A 197	-15.022	4.835	45.726	1.00	19.70	A C
	ATOM 6534 O	THR A 197	-14.532	5.964	45.709	1.00	19.73	A O
10	ATOM 6535 N	LYS A 198	-14.320	3.734	45.480	1.00	18.70	A N
	ATOM 6536 CA	LYS A 198	-12.895	3.773	45.164	1.00	20.70	A C
	ATOM 6537 CB	LYS A 198	-12.321	2.354	45.158	1.00	20.27	A C
	ATOM 6538 CG	LYS A 198	-10.822	2.287	44.939	1.00	21.83	A C
	ATOM 6539 CD	LYS A 198	-10.393	0.877	44.552	1.00	24.28	A C
15	ATOM 6540 CE	LYS A 198	-8.880	0.756	44.464	1.00	25.89	A C
	ATOM 6541 NZ	LYS A 198	-8.481	-0.584	43.937	1.00	28.24	A N
	ATOM 6542 C	LYS A 198	-12.646	4.419	43.800	1.00	21.33	A C
	ATOM 6543 O	LYS A 198	-11.809	5.317	43.664	1.00	20.34	A O
	ATOM 6544 N	LEU A 199	-13.377	3.949	42.793	1.00	21.84	A N
20	ATOM 6545 CA	LEU A 199	-13.245	4.469	41.436	1.00	21.69	A C
	ATOM 6546 CB	LEU A 199	-12.977	3.321	40.459	1.00	23.94	A C
	ATOM 6547 CG	LEU A 199	-11.787	2.419	40.793	1.00	25.29	A C
	ATOM 6548 CD1	LEU A 199	-11.612	1.374	39.698	1.00	25.62	A C
	ATOM 6549 CD2	LEU A 199	-10.528	3.263	40.927	1.00	25.82	A C
25	ATOM 6550 C	LEU A 199	-14.497	5.220	41.004	1.00	21.61	A C

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	ATOM 6551 OT1 LEU A 199	-15.506	5.171	41.740	1.00	20.08	A O
	ATOM 6552 OT2 LEU A 199	-14.454	5.846	39.923	1.00	21.69	A O
	ATOM 6613 N1 GSH H 200	-14.550	5.015	25.946	1.00	13.63	H N
	ATOM 6614 CA1 GSH H 200	-15.807	4.471	26.450	1.00	13.25	H C
5	ATOM 6615 C1 GSH H 200	-16.630	5.539	27.221	1.00	12.75	H C
	ATOM 6616 O11 GSH H 200	-16.085	6.603	27.529	1.00	12.96	H O
	ATOM 6617 O12 GSH H 200	-17.891	5.250	27.492	1.00	15.28	H O
	ATOM 6618 CB1 GSH H 200	-15.460	3.288	27.375	1.00	13.02	H C
	ATOM 6619 CG1 GSH H 200	-16.582	2.234	27.492	1.00	13.79	H C
10	ATOM 6620 CD1 GSH H 200	-16.071	1.156	28.480	1.00	15.77	H C
	ATOM 6621 OE1 GSH H 200	-15.102	0.436	28.187	1.00	15.88	H O
	ATOM 6622 N2 GSH H 200	-16.842	0.986	29.567	1.00	14.96	H N
	ATOM 6623 CA2 GSH H 200	-16.537	-0.058	30.558	1.00	16.29	H C
	ATOM 6624 C2 GSH H 200	-17.470	-1.253	30.341	1.00	17.28	H C
15	ATOM 6625 O2 GSH H 200	-18.558	-1.130	29.767	1.00	15.17	H O
	ATOM 6626 CB2 GSH H 200	-16.864	0.452	31.977	1.00	16.12	H C
	ATOM 6627 SG2 GSH H 200	-15.601	1.558	32.669	1.00	16.79	H S
	ATOM 6628 N3 GSH H 200	-16.899	-2.457	30.507	1.00	19.59	H N
	ATOM 6629 CA3 GSH H 200	-17.689	-3.694	30.640	1.00	20.55	H C
20	ATOM 6630 C3 GSH H 200	-17.281	-4.655	29.543	1.00	22.53	H C
	ATOM 6631 O31 GSH H 200	-17.861	-5.761	29.526	1.00	20.65	H O
	ATOM 6632 O32 GSH H 200	-16.398	-4.285	28.728	1.00	22.35	H O
	ATOM 6708 C1 U44 X 201	-13.533	-1.851	34.292	1.00	70.39	X C
	ATOM 6709 C2 U44 X 201	-13.257	-2.563	35.604	1.00	70.70	X C
25	ATOM 6710 C3 U44 X 201	-12.903	-1.371	36.540	1.00	70.14	X C

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	ATOM 6711 C4	U44	X	201	-13.965	-0.313	36.092	1.00	69.11	X	C
	ATOM 6712 C5	U44	X	201	-14.677	-1.086	34.944	1.00	69.81	X	C
	ATOM 6713 C7	U44	X	201	-15.544	-2.216	35.493	1.00	70.48	X	C
	ATOM 6714 O6	U44	X	201	-14.532	-3.138	35.915	1.00	70.45	X	O
5	ATOM 6715 C14	U44	X	201	-13.413	1.005	35.576	1.00	66.59	X	C
	ATOM 6716 C16	U44	X	201	-13.394	2.213	36.191	1.00	62.13	X	C
	ATOM 6717 C18	U44	X	201	-12.818	3.501	35.639	1.00	58.63	X	C
	ATOM 6718 C20	U44	X	201	-12.819	3.574	34.090	1.00	55.24	X	C
	ATOM 6719 C21	U44	X	201	-11.964	4.730	33.525	1.00	50.86	X	C
10	ATOM 6720 C24	U44	X	201	-12.612	6.108	33.730	1.00	48.35	X	C
	ATOM 6721 C27	U44	X	201	-11.669	7.268	33.392	1.00	45.75	X	C
	ATOM 6722 C30	U44	X	201	-12.193	8.608	33.921	1.00	40.82	X	C
	ATOM 6723 O36	U44	X	201	-11.498	3.620	36.106	1.00	60.26	X	O
	ATOM 6724 C39	U44	X	201	-12.884	-1.741	38.072	1.00	70.91	X	C
15	ATOM 6725 C41	U44	X	201	-14.205	-1.601	38.816	1.00	72.25	X	C
	ATOM 6726 C44	U44	X	201	-14.430	-1.700	40.146	1.00	73.15	X	C
	ATOM 6727 C46	U44	X	201	-13.410	-1.976	41.224	1.00	73.77	X	C
	ATOM 6728 C48	U44	X	201	-13.173	-3.470	41.449	1.00	74.30	X	C
	ATOM 6729 C51	U44	X	201	-11.671	-3.799	41.522	1.00	74.31	X	C
20	ATOM 6730 C54	U44	X	201	-11.421	-5.228	42.015	1.00	74.04	X	C
	ATOM 6731 O57	U44	X	201	-10.109	-5.499	42.071	1.00	74.59	X	O
	ATOM 6732 O58	U44	X	201	-12.270	-6.010	42.314	1.00	73.77	X	O
	ATOM 6734 MG+2	MG2	M	902	-10.576	8.691	23.110	1.00	14.30	M	MG+2
	ATOM 6741 OH2	WAT	S	7	-12.220	10.128	23.608	1.00	19.80	S	O
25	ATOM 6742 OH2	WAT	S	8	-9.999	7.991	24.913	1.00	16.06	S	O

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	ATOM 6743 OH2 WAT S	9	-9.577	7.058	22.052	1.00	9.47	S O
	ATOM 6744 OH2 WAT S	10	-11.304	9.428	21.145	1.00	20.89	S O
	ATOM 6745 OH2 WAT S	11	-8.905	9.998	22.706	1.00	6.56	S O
	ATOM 6746 OH2 WAT S	12	-12.342	7.553	23.132	1.00	5.11	S O
5	ATOM 6755 OH2 WAT S	21	-16.321	10.562	33.715	1.00	12.00	S O
	ATOM 6760 OH2 WAT S	26	-22.235	0.646	24.380	1.00	8.59	S O
	ATOM 6790 OH2 WAT S	56	-19.949	3.890	26.386	1.00	14.06	S O
	ATOM 6822 OH2 WAT S	88	-15.088	1.355	23.422	1.00	11.11	S O
	ATOM 6845 OH2 WAT S	112	-14.218	9.379	37.460	1.00	10.60	S O
10	ATOM 6848 OH2 WAT S	115	-30.009	4.031	30.556	1.00	20.47	S O
	ATOM 6856 OH2 WAT S	123	-21.028	9.378	41.645	1.00	13.15	S O
	ATOM 6857 OH2 WAT S	124	-17.894	1.227	22.644	1.00	11.10	S O
	ATOM 6869 OH2 WAT S	136	-13.700	11.068	39.668	1.00	12.06	S O
	ATOM 6873 OH2 WAT S	140	-16.131	8.790	24.586	1.00	10.01	S O
15	ATOM 6881 OH2 WAT S	148	-14.575	-2.288	28.277	1.00	24.82	S O
	ATOM 6908 OH2 WAT S	177	-20.137	2.340	24.117	1.00	8.16	S O
	ATOM 6925 OH2 WAT S	195	-14.246	-0.057	25.568	1.00	26.38	S O
	ATOM 6936 OH2 WAT S	206	-14.383	-0.255	21.039	1.00	21.10	S O
	ATOM 7014 OH2 WAT S	294	-25.323	5.733	36.748	1.00	14.27	S O
20	ATOM 7015 OH2 WAT S	295	-5.015	5.528	25.654	1.00	25.26	S O
	ATOM 7026 OH2 WAT S	306	-12.125	-1.788	22.440	1.00	16.05	S O
	ATOM 7091 OH2 WAT S	374	-19.550	6.899	43.308	1.00	15.60	S O
	ATOM 7153 OH2 WAT S	445	-10.080	-6.158	38.144	1.00	40.05	S O
	ATOM 7166 OH2 WAT S	461	-11.181	-0.389	24.993	1.00	32.17	S O
25	ATOM 7189 OH2 WAT S	489	-11.757	5.269	27.058	1.00	17.40	S O

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	ATOM 7201 OH2 WAT S 504	-21.955	-1.663	40.073	1.00	22.05	S O
	ATOM 7212 OH2 WAT S 521	-17.307	-1.765	21.966	1.00	22.00	S O
	ATOM 7233 OH2 WAT S 545	-7.572	-3.899	31.498	1.00	31.88	S O
	ATOM 7238 OH2 WAT S 550	-16.631	-4.218	44.114	1.00	28.79	S O
5	ATOM 7255 OH2 WAT S 571	-16.386	-5.314	21.770	1.00	19.46	S O
	ATOM 7274 OH2 WAT S 595	-17.930	-3.842	20.217	1.00	18.12	S O
	ATOM 7276 OH2 WAT S 597	-13.769	7.885	25.487	1.00	10.50	S O
	ATOM 7288 OH2 WAT S 616	-12.729	7.435	38.117	1.00	23.58	S O
	ATOM 7322 OH2 WAT S 668	-8.910	2.771	24.376	1.00	47.74	S O
10	ATOM 7353 OH2 WAT S 728	-24.717	0.462	23.216	1.00	26.35	S O
	ATOM 7375 OH2 WAT S 764	-15.374	9.583	31.111	1.00	11.02	S O
	ATOM 7389 OH2 WAT S 820	-9.060	-6.376	26.123	1.00	42.71	S O
	ATOM 7396 OH2 WAT S 831	-23.318	-6.716	23.568	1.00	37.58	S O
	ATOM 7426 OH2 WAT S 901	-21.607	-1.120	45.347	1.00	32.16	S O
15	ATOM 7495 H2 WAT S1295	-10.054	5.104	25.040	1.00	30.17	S O
	ATOM 7535 OH2 WAT S1341	-11.308	-8.312	40.840	1.00	33.98	S O
	ATOM 7536 OH2 WAT S1342	-18.306	-0.785	45.664	1.00	23.47	S O
	ATOM 7548 OH2 WAT S1355	-11.195	6.225	36.412	1.00	22.59	S O
	ATOM 7552 OH2 WAT S1361	-19.290	-9.723	41.426	1.00	33.42	S O
20	ATOM 7553 OH2 WAT S1362	-20.599	-6.591	22.350	1.00	29.05	S O
	ATOM 7559 OH2 WAT S1368	-9.450	1.544	29.448	1.00	32.22	S O
	ATOM 7560 OH2 WAT S1369	-6.410	-0.567	29.306	1.00	38.08	S O
	ATOM 7566 OH2 WAT S1376	-14.934	13.298	41.070	1.00	13.87	S O
	ATOM 7569 OH2 WAT S1380	-17.170	8.649	45.004	1.00	13.87	S O
25	ATOM 7585 OH2 WAT S1398	-13.501	6.967	29.029	1.00	12.91	S O

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ATOM 7586 OH2 WAT S1399 -11.476 -0.026 31.088 1.00 30.86 S O
ATOM 7591 OH2 WAT S1407 -15.761 -4.514 39.356 1.00 51.81 S O
ATOM 7592 OH2 WAT S1408 -15.589 -5.579 35.465 1.00 42.90 S O
ATOM 7593 OH2 WAT S1409 -7.748 -3.886 41.337 1.00 28.05 S O
5 ATOM 7681 OH2 WAT S1560 -14.609 1.320 43.058 1.00 31.74 S O
ATOM 7688 OH2 WAT S1571 -18.720 -5.226 24.140 1.00 37.27 S O
ATOM 7724 OH2 WAT S1614 -7.499 6.183 23.535 1.00 42.36 S O
ATOM 7745 OH2 WAT S1636 -9.600 -1.548 39.202 1.00 43.85 S O

10 Table 7

Three-dimensional structural coordinate of the complex of
human hematopoietic PGDS with calcium, glutathione and
Cibacron Blue

15 ATOM 1690 N TYR A 8 -2.882 -27.583 10.962 1.00 8.07 A
ATOM 1691 CA TYR A 8 -2.803 -26.193 11.399 1.00 8.37 A
ATOM 1692 CB TYR A 8 -1.457 -25.586 10.986 1.00 8.12 A
ATOM 1693 CG TYR A 8 -1.151 -24.248 11.627 1.00 8.19 A
ATOM 1694 CD1 TYR A 8 -1.019 -24.131 13.013 1.00 7.49 A
20 ATOM 1695 CE1 TYR A 8 -0.726 -22.906 13.605 1.00 7.97 A
ATOM 1696 CD2 TYR A 8 -0.983 -23.099 10.850 1.00 8.28 A
ATOM 1697 CE2 TYR A 8 -0.688 -21.869 11.438 1.00 7.81 A
ATOM 1698 CZ TYR A 8 -0.562 -21.783 12.811 1.00 8.21 A
ATOM 1699 OH TYR A 8 -0.268 -20.575 13.381 1.00 8.12 A
25 ATOM 1700 C TYR A 8 -3.932 -25.418 10.728 1.00 8.79 A

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	ATOM 1701	O	TYR A	8	-4.689	-25.979	9.943	1.00	8.57	A
	ATOM 1702	N	PHE A	9	-4.047	-24.134	11.051	1.00	9.51	A
	ATOM 1703	CA	PHE A	9	-5.069	-23.291	10.446	1.00	10.44	A
	ATOM 1704	CB	PHE A	9	-5.179	-21.963	11.191	1.00	10.48	A
5	ATOM 1705	CG	PHE A	9	-5.739	-22.092	12.572	1.00	11.15	A
	ATOM 1706	CD1	PHE A	9	-5.022	-21.633	13.672	1.00	11.38	A
	ATOM 1707	CD2	PHE A	9	-6.976	-22.684	12.776	1.00	10.92	A
	ATOM 1708	CE1	PHE A	9	-5.539	-21.768	14.960	1.00	11.88	A
	ATOM 1709	CE2	PHE A	9	-7.497	-22.823	14.052	1.00	11.75	A
10	ATOM 1710	CZ	PHE A	9	-6.778	-22.364	15.148	1.00	11.23	A
	ATOM 1711	C	PHE A	9	-4.654	-23.010	9.011	1.00	11.01	A
	ATOM 1712	O	PHE A	9	-3.567	-23.405	8.584	1.00	10.55	A
	ATOM 1713	N	ASN A	10	-5.518	-22.325	8.269	1.00	11.11	A
	ATOM 1714	CA	ASN A	10	-5.204	-21.977	6.887	1.00	11.58	A
15	ATOM 1715	CB	ASN A	10	-6.481	-21.836	6.048	1.00	11.02	A
	ATOM 1716	CG	ASN A	10	-6.192	-21.414	4.615	1.00	12.05	A
	ATOM 1717	OD1	ASN A	10	-5.142	-21.747	4.049	1.00	11.74	A
	ATOM 1718	ND2	ASN A	10	-7.130	-20.690	4.012	1.00	12.36	A
	ATOM 1719	C	ASN A	10	-4.439	-20.655	6.889	1.00	11.87	A
20	ATOM 1720	O	ASN A	10	-4.998	-19.591	6.618	1.00	11.89	A
	ATOM 1721	N	MET A	11	-3.163	-20.732	7.252	1.00	12.14	A
	ATOM 1722	CA	MET A	11	-2.281	-19.570	7.276	1.00	12.22	A
	ATOM 1723	CB	MET A	11	-2.681	-18.571	8.391	1.00	13.94	A
	ATOM 1724	CG	MET A	11	-2.627	-19.064	9.826	1.00	16.67	A
25	ATOM 1725	SD	MET A	11	-3.026	-17.743	11.102	1.00	19.82	A

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	ATOM 1726	CE	MET	A	11	-4.782	-17.673	10.947	1.00	19.20	A
	ATOM 1727	C	MET	A	11	-0.849	-20.065	7.455	1.00	11.51	A
	ATOM 1728	O	MET	A	11	-0.619	-21.250	7.759	1.00	10.85	A
	ATOM 1729	N	ARG	A	12	0.109	-19.180	7.208	1.00	9.73	A
5	ATOM 1730	CA	ARG	A	12	1.508	-19.544	7.373	1.00	9.30	A
	ATOM 1731	CB	ARG	A	12	2.419	-18.405	6.880	1.00	9.27	A
	ATOM 1732	CG	ARG	A	12	2.249	-18.071	5.381	1.00	9.28	A
	ATOM 1733	CD	ARG	A	12	3.317	-17.072	4.886	1.00	9.18	A
	ATOM 1734	NE	ARG	A	12	3.265	-15.815	5.625	1.00	9.17	A
10	ATOM 1735	CZ	ARG	A	12	2.303	-14.905	5.491	1.00	9.26	A
	ATOM 1736	NH1	ARG	A	12	1.311	-15.106	4.633	1.00	9.26	A
	ATOM 1737	NH2	ARG	A	12	2.320	-13.806	6.230	1.00	7.97	A
	ATOM 1738	C	ARG	A	12	1.692	-19.802	8.868	1.00	8.69	A
	ATOM 1739	O	ARG	A	12	1.922	-20.936	9.294	1.00	7.11	A
15	ATOM 1740	N	GLY	A	13	1.568	-18.742	9.660	1.00	8.23	A
	ATOM 1741	CA	GLY	A	13	1.686	-18.879	11.102	1.00	8.26	A
	ATOM 1742	C	GLY	A	13	2.843	-19.731	11.591	1.00	7.95	A
	ATOM 1743	O	GLY	A	13	3.942	-19.685	11.038	1.00	8.28	A
	ATOM 1744	N	ARG	A	14	2.587	-20.533	12.620	1.00	8.33	A
20	ATOM 1745	CA	ARG	A	14	3.623	-21.374	13.210	1.00	8.64	A
	ATOM 1746	CB	ARG	A	14	3.284	-21.628	14.676	1.00	10.55	A
	ATOM 1747	CG	ARG	A	14	3.169	-20.337	15.470	1.00	14.00	A
	ATOM 1748	CD	ARG	A	14	2.974	-20.601	16.955	1.00	16.89	A
	ATOM 1749	NE	ARG	A	14	4.069	-20.046	17.745	1.00	20.03	A
25	ATOM 1750	CZ	ARG	A	14	5.312	-20.519	17.739	1.00	20.80	A

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	ATOM 1751	NH1	ARG	A	14	5.629	-21.561	16.988	1.00	22.98	A
	ATOM 1752	NH2	ARG	A	14	6.242	-19.951	18.482	1.00	21.79	A
	ATOM 1753	C	ARG	A	14	3.894	-22.686	12.500	1.00	8.02	A
	ATOM 1754	O	ARG	A	14	4.787	-23.438	12.888	1.00	7.13	A
5	ATOM 1755	N	ALA	A	15	3.136	-22.958	11.445	1.00	7.13	A
	ATOM 1756	CA	ALA	A	15	3.330	-24.197	10.706	1.00	6.67	A
	ATOM 1757	CB	ALA	A	15	1.987	-24.747	10.262	1.00	6.00	A
	ATOM 1758	C	ALA	A	15	4.221	-23.975	9.497	1.00	6.29	A
	ATOM 1759	O	ALA	A	15	4.765	-24.925	8.934	1.00	6.25	A
10	ATOM 1760	N	GLU	A	16	4.383	-22.714	9.106	1.00	6.29	A
	ATOM 1761	CA	GLU	A	16	5.176	-22.402	7.915	1.00	5.84	A
	ATOM 1762	CB	GLU	A	16	5.209	-20.890	7.678	1.00	4.97	A
	ATOM 1763	CG	GLU	A	16	5.524	-20.485	6.235	1.00	5.83	A
	ATOM 1764	CD	GLU	A	16	4.520	-21.037	5.205	1.00	6.62	A
15	ATOM 1765	OE1	GLU	A	16	3.472	-21.597	5.601	1.00	6.92	A
	ATOM 1766	OE2	GLU	A	16	4.782	-20.883	3.984	1.00	6.47	A
	ATOM 1767	C	GLU	A	16	6.597	-22.952	7.940	1.00	5.58	A
	ATOM 1768	O	GLU	A	16	7.085	-23.435	6.912	1.00	6.05	A
	ATOM 1769	N	ILE	A	17	7.260	-22.890	9.095	1.00	5.19	A
20	ATOM 1770	CA	ILE	A	17	8.631	-23.382	9.203	1.00	5.07	A
	ATOM 1771	CB	ILE	A	17	9.222	-23.154	10.658	1.00	4.92	A
	ATOM 1772	CG2	ILE	A	17	8.396	-23.885	11.716	1.00	4.41	A
	ATOM 1773	CG1	ILE	A	17	10.668	-23.634	10.717	1.00	4.64	A
	ATOM 1774	CD1	ILE	A	17	11.531	-23.053	9.616	1.00	5.86	A
25	ATOM 1775	C	ILE	A	17	8.676	-24.858	8.805	1.00	4.81	A

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	ATOM 1776	O	ILE A	17	9.588	-25.305	8.103	1.00	4.95	A
	ATOM 1966	N	TRP A	39	-11.923	-26.095	14.978	1.00	32.28	A
	ATOM 1967	CA	TRP A	39	-10.853	-26.045	15.967	1.00	32.36	A
	ATOM 1968	CB	TRP A	39	-10.353	-24.604	16.130	1.00	32.57	A
5	ATOM 1969	CG	TRP A	39	-9.352	-24.410	17.236	1.00	32.92	A
	ATOM 1970	CD2	TRP A	39	-8.212	-25.232	17.526	1.00	33.08	A
	ATOM 1971	CE2	TRP A	39	-7.565	-24.666	18.648	1.00	33.25	A
	ATOM 1972	CE3	TRP A	39	-7.676	-26.392	16.950	1.00	33.06	A
	ATOM 1973	CD1	TRP A	39	-9.345	-23.408	18.164	1.00	33.31	A
10	ATOM 1974	NE1	TRP A	39	-8.277	-23.554	19.015	1.00	32.95	A
	ATOM 1975	CZ2	TRP A	39	-6.407	-25.220	19.208	1.00	33.30	A
	ATOM 1976	CZ3	TRP A	39	-6.522	-26.944	17.508	1.00	33.28	A
	ATOM 1977	CH2	TRP A	39	-5.902	-26.353	18.627	1.00	33.07	A
	ATOM 1978	C	TRP A	39	-11.305	-26.596	17.323	1.00	32.24	A
15	ATOM 1979	O	TRP A	39	-10.653	-27.471	17.891	1.00	31.88	A
	ATOM 1980	N	PRO A	40	-12.437	-26.098	17.850	1.00	32.29	A
	ATOM 1981	CD	PRO A	40	-13.335	-25.084	17.264	1.00	32.39	A
	ATOM 1982	CA	PRO A	40	-12.953	-26.557	19.147	1.00	32.22	A
	ATOM 1983	CB	PRO A	40	-14.347	-25.943	19.198	1.00	32.41	A
20	ATOM 1984	CG	PRO A	40	-14.155	-24.651	18.462	1.00	32.65	A
	ATOM 1985	C	PRO A	40	-12.975	-28.077	19.343	1.00	31.96	A
	ATOM 1986	O	PRO A	40	-12.489	-28.579	20.355	1.00	31.96	A
	ATOM 1987	N	GLU A	41	-13.527	-28.810	18.382	1.00	31.78	A
	ATOM 1988	CA	GLU A	41	-13.599	-30.263	18.503	1.00	31.71	A
25	ATOM 1989	CB	GLU A	41	-14.590	-30.831	17.477	1.00	32.59	A

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	ATOM 1990	CG	GLU A	41	-16.039	-30.398	17.728	1.00	34.12	A
	ATOM 1991	CD	GLU A	41	-17.008	-30.864	16.651	1.00	34.74	A
	ATOM 1992	OE1	GLU A	41	-18.136	-30.324	16.602	1.00	35.16	A
	ATOM 1993	OE2	GLU A	41	-16.650	-31.762	15.859	1.00	35.71	A
5	ATOM 1994	C	GLU A	41	-12.248	-30.965	18.374	1.00	31.20	A
	ATOM 1995	O	GLU A	41	-12.026	-32.006	18.994	1.00	31.36	A
	ATOM 1996	N	ILE A	42	-11.341	-30.402	17.581	1.00	30.36	A
	ATOM 1997	CA	ILE A	42	-10.024	-31.008	17.404	1.00	29.44	A
	ATOM 1998	CB	ILE A	42	-9.329	-30.477	16.132	1.00	29.45	A
10	ATOM 1999	CG2	ILE A	42	-7.893	-30.971	16.070	1.00	29.10	A
	ATOM 2000	CG1	ILE A	42	-10.098	-30.946	14.896	1.00	29.17	A
	ATOM 2001	CD1	ILE A	42	-9.533	-30.435	13.587	1.00	29.41	A
	ATOM 2002	C	ILE A	42	-9.133	-30.743	18.614	1.00	29.13	A
	ATOM 2003	O	ILE A	42	-8.395	-31.621	19.064	1.00	28.94	A
15	ATOM 2004	N	LYS A	43	-9.215	-29.527	19.140	1.00	28.55	A
	ATOM 2005	CA	LYS A	43	-8.427	-29.129	20.294	1.00	28.30	A
	ATOM 2006	CB	LYS A	43	-8.860	-27.739	20.757	1.00	28.78	A
	ATOM 2007	CG	LYS A	43	-8.047	-27.185	21.911	1.00	29.29	A
	ATOM 2008	CD	LYS A	43	-8.485	-25.778	22.266	1.00	29.95	A
20	ATOM 2009	CE	LYS A	43	-7.585	-25.184	23.332	1.00	30.31	A
	ATOM 2010	NZ	LYS A	43	-7.992	-23.795	23.662	1.00	31.39	A
	ATOM 2011	C	LYS A	43	-8.554	-30.120	21.452	1.00	27.83	A
	ATOM 2012	O	LYS A	43	-7.565	-30.471	22.088	1.00	27.33	A
	ATOM 2052	N	GLY A	49	-3.879	-29.189	23.684	1.00	18.08	A
25	ATOM 2053	CA	GLY A	49	-4.819	-28.316	23.011	1.00	17.77	A

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	ATOM 2054	C	GLY A	49	-4.205	-27.233	22.144	1.00	17.36	A
	ATOM 2055	O	GLY A	49	-4.742	-26.134	22.055	1.00	17.62	A
	ATOM 2056	N	LYS A	50	-3.087	-27.533	21.492	1.00	16.57	A
	ATOM 2057	CA	LYS A	50	-2.444	-26.544	20.635	1.00	15.44	A
5	ATOM 2058	CB	LYS A	50	-1.252	-25.901	21.357	1.00	16.66	A
	ATOM 2059	CG	LYS A	50	-1.576	-25.229	22.697	1.00	19.15	A
	ATOM 2060	CD	LYS A	50	-2.571	-24.078	22.546	1.00	20.62	A
	ATOM 2061	CE	LYS A	50	-2.752	-23.310	23.863	1.00	22.03	A
	ATOM 2062	NZ	LYS A	50	-1.454	-22.751	24.383	1.00	23.09	A
10	ATOM 2063	C	LYS A	50	-1.962	-27.136	19.308	1.00	14.12	A
	ATOM 2064	O	LYS A	50	-1.634	-28.319	19.214	1.00	12.86	A
	ATOM 2065	N	ILE A	51	-1.935	-26.300	18.280	1.00	12.71	A
	ATOM 2066	CA	ILE A	51	-1.442	-26.709	16.976	1.00	11.10	A
	ATOM 2067	CB	ILE A	51	-2.556	-26.696	15.904	1.00	11.18	A
15	ATOM 2068	CG2	ILE A	51	-3.365	-27.995	15.981	1.00	9.64	A
	ATOM 2069	CG1	ILE A	51	-3.448	-25.464	16.085	1.00	11.01	A
	ATOM 2070	CD1	ILE A	51	-4.506	-25.325	15.031	1.00	11.08	A
	ATOM 2071	C	ILE A	51	-0.361	-25.690	16.641	1.00	11.44	A
	ATOM 2072	O	ILE A	51	-0.312	-24.616	17.240	1.00	11.87	A
20	ATOM 2073	N	PRO A	52	0.490	-25.983	15.651	1.00	10.86	A
	ATOM 2074	CD	PRO A	52	1.653	-25.134	15.342	1.00	10.26	A
	ATOM 2075	CA	PRO A	52	0.506	-27.193	14.826	1.00	9.60	A
	ATOM 2076	CB	PRO A	52	1.479	-26.827	13.715	1.00	10.27	A
	ATOM 2077	CG	PRO A	52	2.505	-26.052	14.470	1.00	10.74	A
25	ATOM 2078	C	PRO A	52	0.917	-28.512	15.473	1.00	9.74	A

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	ATOM 2079	O	PRO	A	52	1.654	-28.551	16.457	1.00	9.94	A
	ATOM 2080	N	ILE	A	53	0.429	-29.595	14.890	1.00	9.16	A
	ATOM 2081	CA	ILE	A	53	0.802	-30.928	15.316	1.00	9.11	A
	ATOM 2082	CB	ILE	A	53	-0.356	-31.724	15.961	1.00	9.49	A
5	ATOM 2083	CG2	ILE	A	53	-0.587	-31.248	17.399	1.00	9.33	A
	ATOM 2084	CG1	ILE	A	53	-1.625	-31.588	15.116	1.00	10.59	A
	ATOM 2085	CD1	ILE	A	53	-2.661	-32.627	15.451	1.00	10.74	A
	ATOM 2086	C	ILE	A	53	1.209	-31.624	14.028	1.00	8.87	A
	ATOM 2087	O	ILE	A	53	0.795	-31.217	12.937	1.00	8.80	A
10	ATOM 2147	N	HIS	A	62	4.066	-32.477	18.677	1.00	7.17	A
	ATOM 2148	CA	HIS	A	62	3.585	-31.113	18.831	1.00	7.13	A
	ATOM 2149	CB	HIS	A	62	2.587	-30.991	20.005	1.00	6.95	A
	ATOM 2150	CG	HIS	A	62	3.182	-31.270	21.350	1.00	7.27	A
	ATOM 2151	CD2	HIS	A	62	3.456	-30.449	22.392	1.00	6.74	A
15	ATOM 2152	ND1	HIS	A	62	3.557	-32.535	21.750	1.00	7.14	A
	ATOM 2153	CE1	HIS	A	62	4.030	-32.482	22.982	1.00	7.45	A
	ATOM 2154	NE2	HIS	A	62	3.981	-31.228	23.394	1.00	7.97	A
	ATOM 2155	C	HIS	A	62	4.749	-30.134	19.018	1.00	6.81	A
	ATOM 2156	O	HIS	A	62	5.903	-30.550	19.138	1.00	6.11	A
20	ATOM 2157	N	GLN	A	63	4.416	-28.840	19.036	1.00	6.34	A
	ATOM 2158	CA	GLN	A	63	5.371	-27.738	19.167	1.00	6.36	A
	ATOM 2159	CB	GLN	A	63	6.378	-27.990	20.295	1.00	6.62	A
	ATOM 2160	CG	GLN	A	63	5.846	-27.668	21.677	1.00	6.95	A
	ATOM 2161	CD	GLN	A	63	5.456	-26.197	21.848	1.00	7.39	A
25	ATOM 2162	OE1	GLN	A	63	5.840	-25.338	21.058	1.00	7.03	A

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	ATOM 2163	NE2	GLN A	63	4.702	-25.909	22.906	1.00	7.11	A
	ATOM 2164	C	GLN A	63	6.108	-27.532	17.848	1.00	6.58	A
	ATOM 2165	O	GLN A	63	6.976	-28.325	17.460	1.00	5.65	A
	ATOM 2166	N	SER A	64	5.756	-26.451	17.163	1.00	7.01	A
5	ATOM 2167	CA	SER A	64	6.327	-26.156	15.858	1.00	7.60	A
	ATOM 2168	CB	SER A	64	5.830	-24.788	15.369	1.00	7.93	A
	ATOM 2169	OG	SER A	64	6.500	-23.724	16.016	1.00	10.49	A
	ATOM 2170	C	SER A	64	7.853	-26.230	15.726	1.00	7.47	A
	ATOM 2171	O	SER A	64	8.355	-26.838	14.778	1.00	8.15	A
10	ATOM 2172	N	LEU A	65	8.590	-25.625	16.659	1.00	7.41	A
	ATOM 2173	CA	LEU A	65	10.057	-25.630	16.588	1.00	6.62	A
	ATOM 2174	CB	LEU A	65	10.635	-24.537	17.507	1.00	6.26	A
	ATOM 2175	CG	LEU A	65	10.102	-23.122	17.220	1.00	6.77	A
	ATOM 2176	CD1	LEU A	65	10.889	-22.083	18.008	1.00	7.45	A
15	ATOM 2177	CD2	LEU A	65	10.218	-22.826	15.727	1.00	6.34	A
	ATOM 2178	C	LEU A	65	10.650	-26.997	16.928	1.00	6.30	A
	ATOM 2179	O	LEU A	65	11.690	-27.382	16.393	1.00	5.38	A
	ATOM 2386	N	ASP A	93	15.188	-19.341	18.472	1.00	6.02	A
	ATOM 2387	CA	ASP A	93	14.502	-18.945	19.704	1.00	6.44	A
20	ATOM 2388	CB	ASP A	93	15.115	-19.629	20.926	1.00	6.17	A
	ATOM 2389	CG	ASP A	93	14.656	-21.070	21.084	1.00	6.96	A
	ATOM 2390	OD1	ASP A	93	15.143	-21.748	22.016	1.00	8.03	A
	ATOM 2391	OD2	ASP A	93	13.816	-21.527	20.286	1.00	7.18	A
	ATOM 2392	C	ASP A	93	14.500	-17.427	19.910	1.00	6.65	A
25	ATOM 2393	O	ASP A	93	13.550	-16.869	20.470	1.00	6.96	A

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	ATOM 2394	N	THR A	94	15.558	-16.761	19.467	1.00	6.46	A
	ATOM 2395	CA	THR A	94	15.605	-15.312	19.606	1.00	7.09	A
	ATOM 2396	CB	THR A	94	16.967	-14.767	19.156	1.00	7.44	A
	ATOM 2397	OG1	THR A	94	17.958	-15.187	20.105	1.00	8.81	A
5	ATOM 2398	CG2	THR A	94	16.960	-13.229	19.084	1.00	8.28	A
	ATOM 2399	C	THR A	94	14.457	-14.732	18.760	1.00	6.91	A
	ATOM 2400	O	THR A	94	13.724	-13.845	19.206	1.00	7.60	A
	ATOM 2401	N	LEU A	95	14.271	-15.265	17.559	1.00	6.06	A
	ATOM 2402	CA	LEU A	95	13.195	-14.795	16.687	1.00	6.05	A
10	ATOM 2403	CB	LEU A	95	13.322	-15.419	15.294	1.00	5.72	A
	ATOM 2404	CG	LEU A	95	14.587	-15.000	14.533	1.00	6.19	A
	ATOM 2405	CD1	LEU A	95	14.726	-15.828	13.269	1.00	5.14	A
	ATOM 2406	CD2	LEU A	95	14.531	-13.509	14.208	1.00	6.20	A
	ATOM 2407	C	LEU A	95	11.835	-15.144	17.289	1.00	6.40	A
15	ATOM 2408	O	LEU A	95	10.930	-14.310	17.332	1.00	6.49	A
	ATOM 2409	N	ASP A	96	11.705	-16.367	17.788	1.00	6.39	A
	ATOM 2410	CA	ASP A	96	10.448	-16.806	18.378	1.00	7.84	A
	ATOM 2411	CB	ASP A	96	10.531	-18.280	18.762	1.00	7.75	A
	ATOM 2412	CG	ASP A	96	9.190	-18.956	18.699	1.00	7.99	A
20	ATOM 2413	OD1	ASP A	96	8.526	-18.824	17.650	1.00	8.64	A
	ATOM 2414	OD2	ASP A	96	8.805	-19.612	19.685	1.00	7.98	A
	ATOM 2415	C	ASP A	96	10.059	-15.970	19.601	1.00	8.25	A
	ATOM 2416	O	ASP A	96	8.886	-15.648	19.787	1.00	8.44	A
	ATOM 2417	N	ASP A	97	11.049	-15.622	20.422	1.00	8.47	A
25	ATOM 2418	CA	ASP A	97	10.810	-14.799	21.601	1.00	9.21	A

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	ATOM 2419	CB	ASP	A	97	12.129	-14.473	22.322	1.00	9.43	A
	ATOM 2420	CG	ASP	A	97	12.692	-15.652	23.121	1.00	10.37	A
	ATOM 2421	OD1	ASP	A	97	13.867	-15.570	23.540	1.00	10.72	A
	ATOM 2422	OD2	ASP	A	97	11.974	-16.651	23.342	1.00	11.19	A
5	ATOM 2423	C	ASP	A	97	10.145	-13.487	21.161	1.00	9.58	A
	ATOM 2424	O	ASP	A	97	9.120	-13.097	21.709	1.00	9.77	A
	ATOM 2425	N	PHE	A	98	10.726	-12.812	20.172	1.00	9.72	A
	ATOM 2426	CA	PHE	A	98	10.162	-11.551	19.712	1.00	9.93	A
	ATOM 2427	CB	PHE	A	98	11.082	-10.888	18.683	1.00	10.00	A
10	ATOM 2428	CG	PHE	A	98	10.641	-9.507	18.285	1.00	10.18	A
	ATOM 2429	CD1	PHE	A	98	10.605	-8.476	19.222	1.00	10.49	A
	ATOM 2430	CD2	PHE	A	98	10.236	-9.246	16.979	1.00	10.06	A
	ATOM 2431	CE1	PHE	A	98	10.164	-7.197	18.861	1.00	10.61	A
	ATOM 2432	CE2	PHE	A	98	9.798	-7.979	16.612	1.00	10.38	A
15	ATOM 2433	CZ	PHE	A	98	9.762	-6.954	17.551	1.00	10.19	A
	ATOM 2434	C	PHE	A	98	8.754	-11.721	19.126	1.00	10.12	A
	ATOM 2435	O	PHE	A	98	7.838	-10.967	19.459	1.00	9.57	A
	ATOM 2436	N	MET	A	99	8.572	-12.723	18.273	1.00	10.66	A
	ATOM 2437	CA	MET	A	99	7.266	-12.956	17.675	1.00	11.35	A
20	ATOM 2438	CB	MET	A	99	7.319	-14.137	16.697	1.00	11.47	A
	ATOM 2439	CG	MET	A	99	8.239	-13.935	15.491	1.00	11.14	A
	ATOM 2440	SD	MET	A	99	7.912	-12.430	14.557	1.00	11.29	A
	ATOM 2441	CE	MET	A	99	6.373	-12.849	13.740	1.00	10.00	A
	ATOM 2442	C	MET	A	99	6.198	-13.223	18.745	1.00	12.00	A
25	ATOM 2443	O	MET	A	99	5.052	-12.804	18.596	1.00	12.28	A

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	ATOM 2444	N	SER A 100	6.562	-13.909	19.823	1.00	12.46	A
	ATOM 2445	CA	SER A 100	5.579	-14.189	20.865	1.00	13.62	A
	ATOM 2446	CB	SER A 100	6.092	-15.288	21.808	1.00	13.99	A
	ATOM 2447	OG	SER A 100	6.241	-16.513	21.108	1.00	15.53	A
5	ATOM 2448	C	SER A 100	5.181	-12.942	21.666	1.00	13.94	A
	ATOM 2449	O	SER A 100	4.196	-12.971	22.400	1.00	14.47	A
	ATOM 2450	N	CYS A 101	5.935	-11.853	21.520	1.00	14.58	A
	ATOM 2451	CA	CYS A 101	5.634	-10.596	22.222	1.00	15.68	A
	ATOM 2452	CB	CYS A 101	6.759	-9.571	22.047	1.00	16.12	A
10	ATOM 2453	SG	CYS A 101	8.291	-9.874	22.933	1.00	20.40	A
	ATOM 2454	C	CYS A 101	4.362	-9.950	21.693	1.00	15.48	A
	ATOM 2455	O	CYS A 101	3.715	-9.184	22.404	1.00	15.75	A
	ATOM 2456	N	PHE A 102	4.012	-10.245	20.445	1.00	15.64	A
	ATOM 2457	CA	PHE A 102	2.825	-9.646	19.849	1.00	15.94	A
15	ATOM 2458	CB	PHE A 102	2.898	-9.712	18.321	1.00	14.57	A
	ATOM 2459	CG	PHE A 102	4.035	-8.929	17.734	1.00	13.99	A
	ATOM 2460	CD1	PHE A 102	5.336	-9.428	17.770	1.00	12.96	A
	ATOM 2461	CD2	PHE A 102	3.812	-7.684	17.158	1.00	13.28	A
	ATOM 2462	CE1	PHE A 102	6.393	-8.701	17.243	1.00	12.46	A
20	ATOM 2463	CE2	PHE A 102	4.865	-6.949	16.628	1.00	13.41	A
	ATOM 2464	CZ	PHE A 102	6.159	-7.459	16.671	1.00	12.82	A
	ATOM 2465	C	PHE A 102	1.529	-10.290	20.321	1.00	16.74	A
	ATOM 2466	O	PHE A 102	1.422	-11.517	20.399	1.00	16.41	A
	ATOM 2467	N	PRO A 103	0.523	-9.460	20.642	1.00	17.53	A
25	ATOM 2468	CD	PRO A 103	0.599	-7.989	20.671	1.00	17.55	A

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	ATOM 2469	CA	PRO A 103	-0.791	-9.916	21.112	1.00	18.81	A
	ATOM 2470	CB	PRO A 103	-1.372	-8.658	21.748	1.00	18.35	A
	ATOM 2471	CG	PRO A 103	-0.855	-7.591	20.841	1.00	17.64	A
	ATOM 2472	C	PRO A 103	-1.646	-10.424	19.954	1.00	19.69	A
5	ATOM 2473	O	PRO A 103	-2.663	-9.827	19.613	1.00	20.09	A
	ATOM 2474	N	TRP A 104	-1.221	-11.527	19.353	1.00	21.16	A
	ATOM 2475	CA	TRP A 104	-1.925	-12.097	18.215	1.00	22.57	A
	ATOM 2476	CB	TRP A 104	-1.215	-13.364	17.740	1.00	22.05	A
	ATOM 2477	CG	TRP A 104	0.208	-13.135	17.325	1.00	22.03	A
10	ATOM 2478	CD2	TRP A 104	0.666	-12.577	16.085	1.00	22.05	A
	ATOM 2479	CE2	TRP A 104	2.076	-12.530	16.144	1.00	22.03	A
	ATOM 2480	CE3	TRP A 104	0.022	-12.110	14.931	1.00	21.92	A
	ATOM 2481	CD1	TRP A 104	1.324	-13.393	18.060	1.00	21.72	A
	ATOM 2482	NE1	TRP A 104	2.449	-13.036	17.360	1.00	21.99	A
15	ATOM 2483	CZ2	TRP A 104	2.856	-12.037	15.092	1.00	22.09	A
	ATOM 2484	CZ3	TRP A 104	0.799	-11.618	13.883	1.00	22.10	A
	ATOM 2485	CH2	TRP A 104	2.199	-11.587	13.973	1.00	22.21	A
	ATOM 2486	C	TRP A 104	-3.398	-12.404	18.462	1.00	23.87	A
	ATOM 2487	O	TRP A 104	-4.227	-12.208	17.580	1.00	23.92	A
20	ATOM 2488	N	ALA A 105	-3.725	-12.880	19.658	1.00	25.71	A
	ATOM 2489	CA	ALA A 105	-5.110	-13.223	19.973	1.00	27.71	A
	ATOM 2490	CB	ALA A 105	-5.161	-14.573	20.686	1.00	27.28	A
	ATOM 2491	C	ALA A 105	-5.827	-12.168	20.814	1.00	28.94	A
	ATOM 2492	O	ALA A 105	-6.594	-12.503	21.714	1.00	29.77	A
25	ATOM 2493	N	GLU A 106	-5.580	-10.897	20.527	1.00	30.28	A

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	ATOM 2494	CA	GLU A 106	-6.227	-9.825	21.272	1.00	31.40	A
	ATOM 2495	CB	GLU A 106	-5.290	-8.622	21.389	1.00	31.69	A
	ATOM 2496	CG	GLU A 106	-5.919	-7.415	22.061	1.00	32.04	A
	ATOM 2497	CD	GLU A 106	-6.531	-7.755	23.407	1.00	32.68	A
5	ATOM 2498	OE1	GLU A 106	-5.780	-8.147	24.328	1.00	33.12	A
	ATOM 2499	OE2	GLU A 106	-7.767	-7.636	23.540	1.00	32.39	A
	ATOM 2500	C	GLU A 106	-7.529	-9.410	20.589	1.00	32.24	A
	ATOM 2501	O	GLU A 106	-7.526	-8.979	19.433	1.00	31.93	A
	ATOM 2502	N	LYS A 107	-8.640	-9.545	21.309	1.00	33.40	A
10	ATOM 2503	CA	LYS A 107	-9.951	-9.194	20.768	1.00	34.44	A
	ATOM 2504	CB	LYS A 107	-11.064	-9.645	21.726	1.00	35.12	A
	ATOM 2505	CG	LYS A 107	-11.028	-11.140	22.042	1.00	36.21	A
	ATOM 2506	CD	LYS A 107	-12.355	-11.678	22.594	1.00	36.94	A
	ATOM 2507	CE	LYS A 107	-12.840	-10.921	23.833	1.00	37.48	A
15	ATOM 2508	NZ	LYS A 107	-13.493	-9.618	23.499	1.00	37.90	A
	ATOM 2509	C	LYS A 107	-10.082	-7.702	20.472	1.00	34.49	A
	ATOM 2510	O	LYS A 107	-10.542	-7.319	19.396	1.00	34.58	A
	ATOM 2511	N	LYS A 108	-9.683	-6.860	21.421	1.00	34.77	A
	ATOM 2512	CA	LYS A 108	-9.755	-5.416	21.208	1.00	34.85	A
20	ATOM 2513	CB	LYS A 108	-9.397	-4.654	22.488	1.00	35.43	A
	ATOM 2514	CG	LYS A 108	-10.511	-4.602	23.526	1.00	36.43	A
	ATOM 2515	CD	LYS A 108	-10.639	-5.902	24.298	1.00	37.04	A
	ATOM 2516	CE	LYS A 108	-9.476	-6.082	25.262	1.00	37.43	A
	ATOM 2517	NZ	LYS A 108	-9.527	-7.411	25.947	1.00	37.89	A
25	ATOM 2518	C	LYS A 108	-8.796	-5.016	20.088	1.00	34.70	A

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	ATOM 2519	O	LYS A 108	-7.578	-5.103	20.239	1.00	34.50	A
	ATOM 2520	N	GLN A 109	-9.359	-4.575	18.968	1.00	34.41	A
	ATOM 2521	CA	GLN A 109	-8.575	-4.174	17.806	1.00	34.31	A
	ATOM 2522	CB	GLN A 109	-9.511	-3.809	16.651	1.00	35.11	A
5	ATOM 2523	CG	GLN A 109	-8.806	-3.584	15.327	1.00	36.38	A
	ATOM 2524	CD	GLN A 109	-8.007	-4.800	14.893	1.00	37.34	A
	ATOM 2525	OE1	GLN A 109	-8.525	-5.922	14.858	1.00	37.88	A
	ATOM 2526	NE2	GLN A 109	-6.737	-4.586	14.560	1.00	37.71	A
	ATOM 2527	C	GLN A 109	-7.632	-3.006	18.082	1.00	33.82	A
10	ATOM 2528	O	GLN A 109	-6.437	-3.086	17.802	1.00	33.77	A
	ATOM 2529	N	ASP A 110	-8.178	-1.921	18.621	1.00	33.24	A
	ATOM 2530	CA	ASP A 110	-7.393	-0.731	18.926	1.00	32.17	A
	ATOM 2531	CB	ASP A 110	-8.290	0.339	19.561	1.00	33.29	A
	ATOM 2532	CG	ASP A 110	-9.147	-0.208	20.689	1.00	34.12	A
15	ATOM 2533	OD1	ASP A 110	-8.607	-0.469	21.785	1.00	34.82	A
	ATOM 2534	OD2	ASP A 110	-10.365	-0.383	20.474	1.00	35.05	A
	ATOM 2535	C	ASP A 110	-6.217	-1.045	19.845	1.00	30.99	A
	ATOM 2536	O	ASP A 110	-5.103	-0.561	19.626	1.00	30.41	A
	ATOM 2537	N	VAL A 111	-6.469	-1.852	20.870	1.00	29.43	A
20	ATOM 2538	CA	VAL A 111	-5.430	-2.236	21.815	1.00	28.27	A
	ATOM 2539	CB	VAL A 111	-6.010	-3.086	22.964	1.00	28.68	A
	ATOM 2540	CG1	VAL A 111	-4.891	-3.532	23.899	1.00	28.43	A
	ATOM 2541	CG2	VAL A 111	-7.061	-2.285	23.718	1.00	28.82	A
	ATOM 2542	C	VAL A 111	-4.373	-3.061	21.089	1.00	27.11	A
25	ATOM 2543	O	VAL A 111	-3.176	-2.848	21.258	1.00	26.42	A

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	ATOM 2544	N	LYS A 112	-4.832	-4.005	20.276	1.00	26.09	A
	ATOM 2545	CA	LYS A 112	-3.936	-4.866	19.518	1.00	25.03	A
	ATOM 2546	CB	LYS A 112	-4.754	-5.880	18.717	1.00	25.17	A
	ATOM 2547	CG	LYS A 112	-3.932	-6.879	17.927	1.00	25.45	A
5	ATOM 2548	CD	LYS A 112	-4.832	-7.932	17.297	1.00	25.91	A
	ATOM 2549	CE	LYS A 112	-4.021	-8.973	16.535	1.00	26.40	A
	ATOM 2550	NZ	LYS A 112	-4.889	-10.025	15.934	1.00	26.69	A
	ATOM 2551	C	LYS A 112	-3.055	-4.044	18.580	1.00	24.09	A
	ATOM 2552	O	LYS A 112	-1.832	-4.200	18.567	1.00	23.73	A
10	ATOM 2553	N	GLU A 113	-3.685	-3.161	17.810	1.00	22.88	A
	ATOM 2554	CA	GLU A 113	-2.980	-2.314	16.853	1.00	22.08	A
	ATOM 2555	CB	GLU A 113	-3.993	-1.498	16.036	1.00	23.03	A
	ATOM 2556	CG	GLU A 113	-3.394	-0.676	14.915	1.00	24.94	A
	ATOM 2557	CD	GLU A 113	-4.453	-0.101	13.976	1.00	26.15	A
15	ATOM 2558	OE1	GLU A 113	-5.181	-0.894	13.332	1.00	26.50	A
	ATOM 2559	OE2	GLU A 113	-4.556	1.142	13.881	1.00	27.05	A
	ATOM 2560	C	GLU A 113	-1.973	-1.383	17.532	1.00	20.78	A
	ATOM 2561	O	GLU A 113	-0.874	-1.162	17.022	1.00	19.80	A
	ATOM 2562	N	GLN A 114	-2.345	-0.839	18.684	1.00	19.79	A
20	ATOM 2563	CA	GLN A 114	-1.450	0.047	19.406	1.00	19.27	A
	ATOM 2564	CB	GLN A 114	-2.154	0.632	20.634	1.00	20.01	A
	ATOM 2565	CG	GLN A 114	-1.301	1.615	21.423	1.00	21.19	A
	ATOM 2566	CD	GLN A 114	-0.997	2.890	20.650	1.00	22.15	A
	ATOM 2567	OE1	GLN A 114	-0.144	3.681	21.059	1.00	23.10	A
25	ATOM 2568	NE2	GLN A 114	-1.699	3.102	19.536	1.00	21.70	A

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	ATOM 2569	C	GLN A 114	-0.188	-0.709	19.838	1.00	18.22	A
	ATOM 2570	O	GLN A 114	0.927	-0.242	19.604	1.00	17.80	A
	ATOM 2571	N	MET A 115	-0.365	-1.877	20.452	1.00	17.56	A
	ATOM 2572	CA	MET A 115	0.769	-2.676	20.908	1.00	17.24	A
5	ATOM 2573	CB	MET A 115	0.290	-3.905	21.693	1.00	19.31	A
	ATOM 2574	CG	MET A 115	1.431	-4.735	22.269	1.00	21.86	A
	ATOM 2575	SD	MET A 115	0.923	-5.795	23.655	1.00	26.35	A
	ATOM 2576	CE	MET A 115	0.941	-4.589	25.027	1.00	25.28	A
	ATOM 2577	C	MET A 115	1.655	-3.122	19.744	1.00	15.84	A
10	ATOM 2578	O	MET A 115	2.882	-3.125	19.860	1.00	15.55	A
	ATOM 2579	N	PHE A 116	1.035	-3.509	18.632	1.00	14.07	A
	ATOM 2580	CA	PHE A 116	1.786	-3.928	17.452	1.00	13.26	A
	ATOM 2581	CB	PHE A 116	0.845	-4.301	16.300	1.00	12.53	A
	ATOM 2582	CG	PHE A 116	0.588	-5.775	16.176	1.00	12.20	A
15	ATOM 2583	CD1	PHE A 116	-0.130	-6.453	17.154	1.00	12.43	A
	ATOM 2584	CD2	PHE A 116	1.076	-6.489	15.089	1.00	12.72	A
	ATOM 2585	CE1	PHE A 116	-0.360	-7.817	17.052	1.00	12.44	A
	ATOM 2586	CE2	PHE A 116	0.851	-7.864	14.974	1.00	12.31	A
	ATOM 2587	CZ	PHE A 116	0.131	-8.526	15.960	1.00	12.74	A
20	ATOM 2588	C	PHE A 116	2.677	-2.775	17.002	1.00	12.47	A
	ATOM 2589	O	PHE A 116	3.870	-2.948	16.773	1.00	12.52	A
	ATOM 2876	N	TYR A 152	13.612	-19.507	9.014	1.00	7.45	A
	ATOM 2877	CA	TYR A 152	12.780	-18.882	10.032	1.00	7.80	A
	ATOM 2878	CB	TYR A 152	13.127	-19.416	11.419	1.00	7.71	A
25	ATOM 2879	CG	TYR A 152	11.963	-19.316	12.386	1.00	8.94	A

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	ATOM 2880	CD1 TYR A 152	10.717	-19.858	12.063	1.00	9.56	A
	ATOM 2881	CE1 TYR A 152	9.649	-19.802	12.961	1.00	9.81	A
	ATOM 2882	CD2 TYR A 152	12.110	-18.706	13.630	1.00	9.51	A
	ATOM 2883	CE2 TYR A 152	11.050	-18.642	14.534	1.00	9.37	A
5	ATOM 2884	CZ TYR A 152	9.828	-19.197	14.191	1.00	10.01	A
	ATOM 2885	OH TYR A 152	8.787	-19.193	15.101	1.00	10.22	A
	ATOM 2886	C TYR A 152	12.871	-17.368	10.032	1.00	7.80	A
	ATOM 2887	O TYR A 152	11.906	-16.685	10.363	1.00	7.64	A
	ATOM 2888	N TRP A 153	14.037	-16.848	9.671	1.00	7.83	A
10	ATOM 2889	CA TRP A 153	14.217	-15.409	9.615	1.00	8.29	A
	ATOM 2890	CB TRP A 153	15.675	-15.058	9.323	1.00	8.19	A
	ATOM 2891	CG TRP A 153	15.826	-13.715	8.694	1.00	8.54	A
	ATOM 2892	CD2 TRP A 153	15.414	-12.464	9.247	1.00	8.88	A
	ATOM 2893	CE2 TRP A 153	15.716	-11.467	8.299	1.00	8.91	A
15	ATOM 2894	CE3 TRP A 153	14.816	-12.087	10.458	1.00	9.75	A
	ATOM 2895	CD1 TRP A 153	16.348	-13.438	7.466	1.00	8.71	A
	ATOM 2896	NE1 TRP A 153	16.285	-12.087	7.219	1.00	9.04	A
	ATOM 2897	CZ2 TRP A 153	15.440	-10.111	8.519	1.00	9.95	A
	ATOM 2898	CZ3 TRP A 153	14.541	-10.734	10.676	1.00	9.92	A
20	ATOM 2899	CH2 TRP A 153	14.855	-9.766	9.708	1.00	9.14	A
	ATOM 2900	C TRP A 153	13.336	-14.871	8.493	1.00	8.23	A
	ATOM 2901	O TRP A 153	12.676	-13.852	8.647	1.00	8.77	A
	ATOM 2902	N GLU A 154	13.336	-15.572	7.364	1.00	8.71	A
	ATOM 2903	CA GLU A 154	12.547	-15.159	6.204	1.00	8.50	A
25	ATOM 2904	CB GLU A 154	12.862	-16.034	4.995	1.00	8.57	A

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	ATOM 2905	CG	GLU A 154	12.336	-15.455	3.679	1.00	9.53	A
	ATOM 2906	CD	GLU A 154	10.920	-15.883	3.350	1.00	8.58	A
	ATOM 2907	OE1	GLU A 154	10.337	-15.318	2.400	1.00	9.21	A
	ATOM 2908	OE2	GLU A 154	10.397	-16.785	4.019	1.00	8.79	A
5	ATOM 2909	C	GLU A 154	11.064	-15.205	6.496	1.00	8.22	A
	ATOM 2910	O	GLU A 154	10.310	-14.309	6.102	1.00	8.84	A
	ATOM 2911	N	ILE A 155	10.650	-16.258	7.191	1.00	7.89	A
	ATOM 2912	CA	ILE A 155	9.254	-16.444	7.547	1.00	6.85	A
	ATOM 2913	CB	ILE A 155	9.041	-17.887	8.105	1.00	7.23	A
10	ATOM 2914	CG2	ILE A 155	7.742	-17.975	8.898	1.00	6.59	A
	ATOM 2915	CG1	ILE A 155	9.067	-18.893	6.939	1.00	7.31	A
	ATOM 2916	CD1	ILE A 155	9.155	-20.382	7.343	1.00	5.54	A
	ATOM 2917	C	ILE A 155	8.816	-15.378	8.568	1.00	7.33	A
	ATOM 2918	O	ILE A 155	7.801	-14.702	8.375	1.00	6.57	A
15	ATOM 2919	N	CYS A 156	9.601	-15.196	9.628	1.00	7.49	A
	ATOM 2920	CA	CYS A 156	9.245	-14.209	10.638	1.00	7.46	A
	ATOM 2921	CB	CYS A 156	10.227	-14.252	11.818	1.00	7.91	A
	ATOM 2922	SG	CYS A 156	10.226	-15.769	12.755	1.00	8.41	A
	ATOM 2923	C	CYS A 156	9.230	-12.799	10.029	1.00	7.56	A
20	ATOM 2924	O	CYS A 156	8.238	-12.075	10.148	1.00	7.15	A
	ATOM 2925	N	SER A 157	10.296	-12.427	9.319	1.00	7.31	A
	ATOM 2926	CA	SER A 157	10.345	-11.095	8.733	1.00	7.15	A
	ATOM 2927	CB	SER A 157	11.739	-10.802	8.137	1.00	6.90	A
	ATOM 2928	OG	SER A 157	12.045	-11.626	7.027	1.00	5.72	A
25	ATOM 2929	C	SER A 157	9.226	-10.893	7.706	1.00	7.42	A

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	ATOM 2930	O	SER A 157	8.700	-9.793	7.591	1.00	7.72	A
	ATOM 2931	N	THR A 158	8.831	-11.938	6.980	1.00	7.58	A
	ATOM 2932	CA	THR A 158	7.744	-11.762	6.012	1.00	8.17	A
	ATOM 2933	CB	THR A 158	7.434	-13.070	5.248	1.00	8.62	A
5	ATOM 2934	OG1	THR A 158	8.325	-13.172	4.128	1.00	9.05	A
	ATOM 2935	CG2	THR A 158	5.989	-13.090	4.742	1.00	8.43	A
	ATOM 2936	C	THR A 158	6.491	-11.257	6.733	1.00	8.44	A
	ATOM 2937	O	THR A 158	5.843	-10.317	6.278	1.00	7.98	A
	ATOM 2938	N	THR A 159	6.178	-11.848	7.881	1.00	8.66	A
10	ATOM 2939	CA	THR A 159	5.008	-11.421	8.630	1.00	9.74	A
	ATOM 2940	CB	THR A 159	4.661	-12.441	9.728	1.00	11.00	A
	ATOM 2941	OG1	THR A 159	4.147	-13.633	9.113	1.00	11.94	A
	ATOM 2942	CG2	THR A 159	3.603	-11.874	10.663	1.00	11.12	A
	ATOM 2943	C	THR A 159	5.136	-10.016	9.248	1.00	9.29	A
15	ATOM 2944	O	THR A 159	4.201	-9.222	9.163	1.00	9.32	A
	ATOM 2945	N	LEU A 160	6.287	-9.707	9.850	1.00	9.10	A
	ATOM 2946	CA	LEU A 160	6.509	-8.394	10.464	1.00	8.76	A
	ATOM 2947	CB	LEU A 160	7.887	-8.342	11.143	1.00	8.08	A
	ATOM 2948	CG	LEU A 160	8.152	-9.296	12.318	1.00	8.40	A
20	ATOM 2949	CD1	LEU A 160	9.616	-9.250	12.706	1.00	7.66	A
	ATOM 2950	CD2	LEU A 160	7.259	-8.925	13.491	1.00	7.69	A
	ATOM 2951	C	LEU A 160	6.424	-7.279	9.417	1.00	8.80	A
	ATOM 2952	O	LEU A 160	5.912	-6.192	9.691	1.00	8.81	A
	ATOM 2953	N	LEU A 161	6.946	-7.553	8.226	1.00	9.13	A
25	ATOM 2954	CA	LEU A 161	6.921	-6.586	7.131	1.00	9.84	A

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	ATOM 2955	CB	LEU A 161	7.637	-7.159	5.905	1.00	9.15	A
	ATOM 2956	CG	LEU A 161	9.144	-6.881	5.882	1.00	9.55	A
	ATOM 2957	CD1	LEU A 161	9.822	-7.612	4.700	1.00	9.05	A
	ATOM 2958	CD2	LEU A 161	9.351	-5.388	5.757	1.00	8.83	A
5	ATOM 2959	C	LEU A 161	5.495	-6.184	6.768	1.00	10.43	A
	ATOM 2960	O	LEU A 161	5.262	-5.090	6.249	1.00	10.78	A
	ATOM 2961	N	VAL A 162	4.542	-7.068	7.055	1.00	10.57	A
	ATOM 2962	CA	VAL A 162	3.137	-6.794	6.776	1.00	11.31	A
	ATOM 2963	CB	VAL A 162	2.244	-8.045	7.041	1.00	11.09	A
10	ATOM 2964	CG1	VAL A 162	0.770	-7.682	6.916	1.00	12.11	A
	ATOM 2965	CG2	VAL A 162	2.585	-9.147	6.047	1.00	11.31	A
	ATOM 2966	C	VAL A 162	2.660	-5.648	7.662	1.00	11.94	A
	ATOM 2967	O	VAL A 162	1.909	-4.789	7.214	1.00	12.85	A
	ATOM 2968	N	PHE A 163	3.104	-5.622	8.916	1.00	12.19	A
15	ATOM 2969	CA	PHE A 163	2.681	-4.561	9.825	1.00	12.54	A
	ATOM 2970	CB	PHE A 163	2.500	-5.112	11.239	1.00	13.07	A
	ATOM 2971	CG	PHE A 163	1.527	-6.248	11.321	1.00	14.49	A
	ATOM 2972	CD1	PHE A 163	1.959	-7.555	11.156	1.00	14.30	A
	ATOM 2973	CD2	PHE A 163	0.168	-6.007	11.532	1.00	14.47	A
20	ATOM 2974	CE1	PHE A 163	1.058	-8.618	11.197	1.00	15.26	A
	ATOM 2975	CE2	PHE A 163	-0.743	-7.061	11.574	1.00	15.43	A
	ATOM 2976	CZ	PHE A 163	-0.297	-8.371	11.406	1.00	14.83	A
	ATOM 2977	C	PHE A 163	3.625	-3.362	9.868	1.00	12.48	A
	ATOM 2978	O	PHE A 163	3.233	-2.280	10.305	1.00	12.19	A
25	ATOM 3252	N	THR A 197	-2.372	-16.130	2.207	1.00	8.89	A

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	ATOM 3253	CA	THR A 197	-3.090	-15.716	3.399	1.00	9.12	A
	ATOM 3254	CB	THR A 197	-3.159	-16.854	4.438	1.00	8.54	A
	ATOM 3255	OG1	THR A 197	-1.826	-17.241	4.803	1.00	7.22	A
	ATOM 3256	CG2	THR A 197	-3.891	-18.055	3.859	1.00	8.20	A
5	ATOM 3257	C	THR A 197	-2.349	-14.557	4.045	1.00	10.07	A
	ATOM 3258	O	THR A 197	-1.153	-14.380	3.829	1.00	9.98	A
	ATOM 3259	N	LYS A 198	-3.063	-13.756	4.821	1.00	11.83	A
	ATOM 3260	CA	LYS A 198	-2.431	-12.648	5.525	1.00	14.16	A
	ATOM 3261	CB	LYS A 198	-3.407	-11.497	5.746	1.00	14.77	A
10	ATOM 3262	CG	LYS A 198	-2.803	-10.367	6.571	1.00	16.50	A
	ATOM 3263	CD	LYS A 198	-3.868	-9.483	7.196	1.00	17.64	A
	ATOM 3264	CE	LYS A 198	-3.217	-8.361	8.008	1.00	18.15	A
	ATOM 3265	NZ	LYS A 198	-4.215	-7.462	8.646	1.00	18.92	A
	ATOM 3266	C	LYS A 198	-2.042	-13.213	6.882	1.00	15.13	A
15	ATOM 3267	O	LYS A 198	-2.869	-13.236	7.788	1.00	17.31	A
	ATOM 3268	N	LEU A 199	-0.803	-13.670	7.005	1.00	14.65	A
	ATOM 3269	CA	LEU A 199	-0.257	-14.254	8.234	1.00	13.81	A
	ATOM 3270	CB	LEU A 199	-1.137	-13.966	9.468	1.00	15.00	A
	ATOM 3271	CG	LEU A 199	-1.354	-12.517	9.953	1.00	15.52	A
20	ATOM 3272	CD1	LEU A 199	-2.352	-12.514	11.110	1.00	15.65	A
	ATOM 3273	CD2	LEU A 199	-0.032	-11.901	10.400	1.00	16.55	A
	ATOM 3274	C	LEU A 199	-0.078	-15.770	8.070	1.00	13.40	A
	ATOM 3275	O	LEU A 199	0.673	-16.360	8.862	1.00	12.28	A
	ATOM 3276	OXT	LEU A 199	-0.695	-16.347	7.147	1.00	12.25	A
25	ATOM 6573	N1	GSH F 200	4.240	-22.620	20.817	1.00	44.60	F

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	ATOM 6574	CA1	GSH	F	200	3.413	-23.575	20.073	1.00	44.99	F
	ATOM 6575	C1	GSH	F	200	4.146	-24.142	18.822	1.00	44.16	F
	ATOM 6576	O11	GSH	F	200	5.277	-23.724	18.545	1.00	44.01	F
	ATOM 6577	O12	GSH	F	200	3.502	-25.050	18.113	1.00	43.49	F
5	ATOM 6578	CB1	GSH	F	200	2.101	-22.895	19.661	1.00	45.74	F
	ATOM 6579	CG1	GSH	F	200	1.180	-22.538	20.853	1.00	46.69	F
	ATOM 6580	CD1	GSH	F	200	0.010	-21.712	20.254	1.00	47.11	F
	ATOM 6581	OE1	GSH	F	200	-0.142	-20.530	20.586	1.00	47.97	F
	ATOM 6582	N2	GSH	F	200	-0.754	-22.340	19.334	1.00	47.00	F
10	ATOM 6583	CA2	GSH	F	200	-1.817	-21.594	18.641	1.00	46.63	F
	ATOM 6584	C2	GSH	F	200	-3.172	-22.214	18.985	1.00	46.78	F
	ATOM 6585	O2	GSH	F	200	-3.381	-23.428	18.891	1.00	46.26	F
	ATOM 6586	CB2	GSH	F	200	-1.659	-21.704	17.108	1.00	46.61	F
	ATOM 6587	SG2	GSH	F	200	-0.726	-20.334	16.354	1.00	45.55	F
15	ATOM 6588	N3	GSH	F	200	-4.138	-21.341	19.347	1.00	47.03	F
	ATOM 6589	CA3	GSH	F	200	-5.549	-21.727	19.555	1.00	47.63	F
	ATOM 6590	C3	GSH	F	200	-5.805	-21.983	21.029	1.00	47.96	F
	ATOM 6591	O31	GSH	F	200	-6.963	-22.325	21.339	1.00	48.33	F
	ATOM 6592	O32	GSH	F	200	-4.849	-21.855	21.833	1.00	48.13	F
20	ATOM 6684	C1	CBD	V	201	1.320	-16.944	18.446	1.00	55.65	V
	ATOM 6685	SA	CBD	V	201	0.790	-17.122	20.115	1.00	56.02	V
	ATOM 6686	O1A	CBD	V	201	1.575	-18.205	20.799	1.00	55.76	V
	ATOM 6687	O2A	CBD	V	201	-0.636	-17.464	19.966	1.00	55.91	V
	ATOM 6688	O3A	CBD	V	201	1.221	-15.829	20.717	1.00	55.92	V
25	ATOM 6689	C2	CBD	V	201	2.711	-17.027	18.129	1.00	55.38	V

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	ATOM 6690	N2	CBD V 201	3.702	-17.265	19.274	1.00	55.19	V
	ATOM 6691	C3	CBD V 201	3.112	-16.894	16.760	1.00	55.20	V
	ATOM 6692	C4	CBD V 201	4.532	-16.974	16.323	1.00	54.93	V
	ATOM 6693	O4	CBD V 201	5.374	-17.167	17.212	1.00	55.39	V
5	ATOM 6694	C5	CBD V 201	5.017	-16.849	14.925	1.00	54.45	V
	ATOM 6695	C6	CBD V 201	6.495	-16.945	14.509	1.00	54.14	V
	ATOM 6696	C7	CBD V 201	6.812	-16.806	13.140	1.00	53.94	V
	ATOM 6697	C8	CBD V 201	5.803	-16.585	12.172	1.00	53.98	V
	ATOM 6698	C9	CBD V 201	4.432	-16.493	12.529	1.00	54.22	V
10	ATOM 6699	C10	CBD V 201	4.023	-16.624	13.897	1.00	54.48	V
	ATOM 6700	C11	CBD V 201	2.621	-16.543	14.333	1.00	54.89	V
	ATOM 6701	O11	CBD V 201	1.771	-16.353	13.468	1.00	54.55	V
	ATOM 6702	C12	CBD V 201	2.094	-16.666	15.725	1.00	55.45	V
	ATOM 6703	C13	CBD V 201	0.676	-16.584	16.095	1.00	56.18	V
15	ATOM 6704	C14	CBD V 201	0.298	-16.725	17.474	1.00	55.98	V
	ATOM 6705	NB	CBD V 201	-0.387	-16.360	15.063	1.00	57.55	V
	ATOM 6706	CB1	CBD V 201	-4.096	-17.069	15.898	1.00	61.45	V
	ATOM 6707	SB	CBD V 201	-5.117	-18.384	16.588	1.00	62.03	V
	ATOM 6708	O1B	CBD V 201	-5.591	-17.837	17.918	1.00	62.06	V
20	ATOM 6709	O2B	CBD V 201	-4.217	-19.550	16.781	1.00	62.13	V
	ATOM 6710	O3B	CBD V 201	-6.221	-18.727	15.629	1.00	61.84	V
	ATOM 6711	CB2	CBD V 201	-4.648	-15.806	15.457	1.00	61.61	V
	ATOM 6712	CB3	CBD V 201	-3.798	-14.783	14.909	1.00	60.85	V
	ATOM 6713	CB4	CBD V 201	-2.415	-14.973	14.785	1.00	59.79	V
25	ATOM 6714	CB5	CBD V 201	-1.838	-16.208	15.214	1.00	59.24	V

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	ATOM 6715	CB6	CBD	V	201	-2.667	-17.266	15.769	1.00	60.28	V
	ATOM 6716	NC	CBD	V	201	-6.100	-15.699	15.626	1.00	62.61	V
	ATOM 6717	NC1	CBD	V	201	-7.272	-13.869	16.843	1.00	64.01	V
	ATOM 6718	CC2	CBD	V	201	-7.958	-12.677	16.830	1.00	64.30	V
5	ATOM 6719	XCL	CBD	V	201	-8.536	-11.955	18.433	1.00	64.97	V
	ATOM 6720	NC3	CBD	V	201	-8.179	-12.086	15.587	1.00	64.60	V
	ATOM 6721	CC4	CBD	V	201	-7.742	-12.647	14.411	1.00	64.72	V
	ATOM 6722	NC5	CBD	V	201	-7.067	-13.826	14.459	1.00	64.27	V
	ATOM 6723	CC6	CBD	V	201	-6.835	-14.427	15.666	1.00	63.60	V
10	ATOM 6724	ND	CBD	V	201	-7.999	-11.990	13.118	1.00	65.16	V
	ATOM 6725	CD1	CBD	V	201	-6.460	-11.914	11.166	1.00	65.80	V
	ATOM 6726	SD	CBD	V	201	-5.663	-10.543	12.000	1.00	66.14	V
	ATOM 6727	O1D	CBD	V	201	-4.963	-11.035	13.249	1.00	66.20	V
	ATOM 6728	O2D	CBD	V	201	-6.740	-9.533	12.229	1.00	66.14	V
15	ATOM 6729	O3D	CBD	V	201	-4.469	-9.967	11.283	1.00	66.06	V
	ATOM 6730	CD2	CBD	V	201	-7.612	-12.553	11.819	1.00	65.58	V
	ATOM 6731	CD3	CBD	V	201	-8.282	-13.667	11.168	1.00	65.50	V
	ATOM 6732	CD4	CBD	V	201	-7.820	-14.138	9.898	1.00	65.62	V
	ATOM 6733	CD5	CBD	V	201	-6.689	-13.516	9.253	1.00	65.58	V
20	ATOM 6734	CD6	CBD	V	201	-6.009	-12.418	9.867	1.00	65.66	V
	ATOM 6736	CA+2	CA2	M	902	10.668	-20.783	23.896	1.00	51.04	M
	ATOM 6737	OH2	WAT	S	1	1.351	-21.691	3.667	1.00	7.98	S
	ATOM 6739	OH2	WAT	S	3	-1.239	-27.422	7.740	1.00	3.33	S
	ATOM 6740	OH2	WAT	S	4	8.134	-25.070	19.531	1.00	9.51	S
25	ATOM 6743	OH2	WAT	S	7	6.599	-20.828	11.162	1.00	4.11	S

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	ATOM 6747	OH2 WAT S	11	5.286	-16.048	7.235	1.00	3.73	S
	ATOM 6751	OH2 WAT S	15	6.780	-21.479	14.227	1.00	6.02	S
	ATOM 6758	OH2 WAT S	22	0.702	-16.833	2.360	1.00	8.75	S
	ATOM 6760	OH2 WAT S	24	7.629	-15.477	2.582	1.00	9.74	S
5	ATOM 6761	OH2 WAT S	25	-2.129	-33.873	12.001	1.00	6.94	S
	ATOM 6772	OH2 WAT S	36	0.027	-13.756	1.035	1.00	15.53	S
	ATOM 6773	OH2 WAT S	37	2.414	-15.170	10.370	1.00	10.38	S
	ATOM 6777	OH2 WAT S	42	9.861	-20.611	21.788	1.00	19.36	S
	ATOM 6782	OH2 WAT S	47	-0.738	-19.696	3.763	1.00	7.26	S
10	ATOM 6786	OH2 WAT S	51	-8.079	-21.562	9.291	1.00	11.54	S
	ATOM 6798	OH2 WAT S	63	11.971	-27.063	20.805	1.00	13.89	S
	ATOM 6799	OH2 WAT S	64	-6.746	-29.289	4.136	1.00	17.17	S
	ATOM 6806	OH2 WAT S	71	2.082	-27.303	18.951	1.00	6.50	S
	ATOM 6808	OH2 WAT S	73	6.370	-34.029	20.049	1.00	7.66	S
15	ATOM 6833	OH2 WAT S	98	-0.925	-29.526	21.487	1.00	8.88	S
	ATOM 6873	OH2 WAT S	138	12.612	-27.001	23.449	1.00	21.34	S
	ATOM 6881	OH2 WAT S	146	1.862	-24.047	27.300	1.00	13.69	S
	ATOM 6900	OH2 WAT S	165	8.353	-19.515	24.914	1.00	21.77	S
	ATOM 6940	OH2 WAT S	205	-5.859	-14.566	5.222	1.00	13.11	S
20	ATOM 6972	OH2 WAT S	237	-2.575	-19.558	21.111	1.00	44.73	S
	ATOM 6992	OH2 WAT S	257	-8.895	-24.364	5.325	1.00	26.95	S
	ATOM 6996	OH2 WAT S	261	4.413	-17.589	25.511	1.00	30.40	S
	ATOM 7000	OH2 WAT S	265	-5.639	-28.605	26.537	1.00	35.00	S
	ATOM 7015	OH2 WAT S	280	-6.647	-16.720	1.613	1.00	29.73	S
25	ATOM 7031	OH2 WAT S	296	13.593	-19.947	25.168	1.00	25.03	S

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	ATOM 7053	OH2 WAT S 318	6.658	-19.330	21.220	1.00	29.42	S
	ATOM 7057	OH2 WAT S 322	7.702	-22.083	20.657	1.00	26.23	S
	ATOM 7060	OH2 WAT S 325	13.812	-24.922	22.589	1.00	25.62	S
	ATOM 7066	OH2 WAT S 331	-3.023	-35.741	20.966	1.00	51.90	S
5	ATOM 7071	OH2 WAT S 336	8.646	-22.439	23.070	1.00	32.36	S
	ATOM 7117	OH2 WAT S 383	-7.864	-19.607	18.001	1.00	49.01	S
	ATOM 7119	OH2 WAT S 385	12.122	-19.312	22.304	1.00	36.04	S
	ATOM 7149	OH2 WAT S 415	4.500	-17.354	9.500	1.00	17.11	S
	ATOM 7151	OH2 WAT S 417	3.003	-10.979	2.789	1.00	8.57	S
10	ATOM 7161	OH2 WAT S 427	1.666	-28.319	21.869	1.00	9.23	S
	ATOM 7173	OH2 WAT S 439	1.707	-26.590	23.994	1.00	20.49	S
	ATOM 7175	OH2 WAT S 441	-7.142	-12.553	6.181	1.00	27.77	S
	ATOM 7217	OH2 WAT S 483	-1.287	-25.245	26.731	1.00	38.16	S
	ATOM 7239	OH2 WAT S 505	8.962	-18.324	22.747	1.00	40.69	S
15	ATOM 7269	OH2 WAT S 535	-8.231	-19.382	10.779	1.00	39.27	S
	ATOM 7291	OH2 WAT S 557	-7.790	-15.423	3.534	1.00	48.88	S
	ATOM 7294	OH2 WAT S 560	-6.131	-17.042	6.655	1.00	28.01	S
	ATOM 7305	OH2 WAT S 571	-5.344	-20.658	29.405	1.00	33.64	S
	ATOM 7319	OH2 WAT S 585	-8.529	-10.641	23.648	1.00	36.23	S
20	ATOM 7335	OH2 WAT S 601	13.245	-24.342	20.045	1.00	20.43	S
	ATOM 7341	OH2 WAT S 607	15.091	-23.061	18.509	1.00	28.00	S
	ATOM 7342	OH2 WAT S 608	2.114	-23.889	24.521	1.00	24.13	S
	ATOM 7354	OH2 WAT S 620	-5.822	-33.782	12.796	1.00	39.40	S
	ATOM 7412	OH2 WAT S 679	-4.210	-15.053	7.903	1.00	7.85	S
25	ATOM 7416	OH2 WAT S 683	-11.812	-20.860	17.588	1.00	35.78	S

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	ATOM 7418	OH2	WAT	S	685	-5.319	-36.445	17.400	1.00	36.65	S
	ATOM 7432	OH2	WAT	S	701	0.414	-10.954	3.856	1.00	3.57	S
	ATOM 7433	OH2	WAT	S	702	3.171	-13.470	2.015	1.00	31.21	S
	ATOM 7518	OH2	WAT	S	792	-6.880	-19.345	1.064	1.00	28.83	S
5	ATOM 7544	OH2	WAT	S	818	-14.589	-21.459	10.093	1.00	28.52	S
	ATOM 7546	OH2	WAT	S	820	-15.291	-27.899	16.026	1.00	38.45	S
	ATOM 7576	OH2	WAT	S	850	4.135	-19.875	21.107	1.00	51.02	S
	ATOM 7581	OH2	WAT	S	855	5.075	-11.173	29.078	1.00	44.63	S
	ATOM 7582	OH2	WAT	S	856	-1.969	-27.093	28.386	1.00	36.21	S
10	ATOM 7590	OH2	WAT	S	864	1.742	-9.916	24.316	1.00	49.81	S
	ATOM 7591	OH2	WAT	S	865	6.598	-16.698	4.969	1.00	27.41	S

Table 8

15 Three-dimensional structural coordinate of the complex of human hematopoietic PGDS with magnesium, glutathione and 4-benzhydryloxy-1-{3-(1H-tetrazol-5-yl)-propyl}piperidine (HQL-79)

20	ATOM 4966	N	TYR	A	8	17.463	-2.741	10.967	1.00	2.30	A
	ATOM 4967	CA	TYR	A	8	16.069	-2.648	11.384	1.00	2.27	A
	ATOM 4968	CB	TYR	A	8	15.463	-1.311	10.947	1.00	1.93	A
	ATOM 4969	CG	TYR	A	8	14.123	-1.007	11.579	1.00	1.75	A
	ATOM 4970	CD1	TYR	A	8	13.996	-0.888	12.962	1.00	1.76	A
25	ATOM 4971	CE1	TYR	A	8	12.771	-0.568	13.551	1.00	1.82	A

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	ATOM 4972	CD2	TYR	A	8	12.987	-0.803	10.792	1.00	1.81	A
	ATOM 4973	CE2	TYR	A	8	11.762	-0.479	11.366	1.00	2.19	A
	ATOM 4974	CZ	TYR	A	8	11.658	-0.360	12.748	1.00	1.84	A
	ATOM 4975	OH	TYR	A	8	10.456	-0.003	13.318	1.00	2.39	A
5	ATOM 4976	C	TYR	A	8	15.320	-3.786	10.709	1.00	2.74	A
	ATOM 4977	O	TYR	A	8	15.902	-4.543	9.939	1.00	2.59	A
	ATOM 4978	N	PHE	A	9	14.033	-3.916	11.011	1.00	3.54	A
	ATOM 4979	CA	PHE	A	9	13.216	-4.945	10.378	1.00	4.12	A
	ATOM 4980	CB	PHE	A	9	11.873	-5.079	11.102	1.00	4.53	A
10	ATOM 4981	CG	PHE	A	9	11.981	-5.579	12.511	1.00	4.71	A
	ATOM 4982	CD1	PHE	A	9	11.552	-4.791	13.577	1.00	5.32	A
	ATOM 4983	CD2	PHE	A	9	12.499	-6.844	12.777	1.00	5.02	A
	ATOM 4984	CE1	PHE	A	9	11.639	-5.256	14.889	1.00	5.60	A
	ATOM 4985	CE2	PHE	A	9	12.589	-7.316	14.085	1.00	5.47	A
15	ATOM 4986	CZ	PHE	A	9	12.158	-6.521	15.142	1.00	5.95	A
	ATOM 4987	C	PHE	A	9	12.946	-4.517	8.936	1.00	4.36	A
	ATOM 4988	O	PHE	A	9	13.277	-3.398	8.532	1.00	4.11	A
	ATOM 4989	N	ASN	A	10	12.354	-5.405	8.146	1.00	4.68	A
	ATOM 4990	CA	ASN	A	10	12.026	-5.046	6.778	1.00	5.42	A
20	ATOM 4991	CB	ASN	A	10	11.933	-6.278	5.880	1.00	5.82	A
	ATOM 4992	CG	ASN	A	10	11.502	-5.933	4.465	1.00	6.24	A
	ATOM 4993	OD1	ASN	A	10	11.787	-4.841	3.954	1.00	6.66	A
	ATOM 4994	ND2	ASN	A	10	10.822	-6.869	3.814	1.00	7.65	A
	ATOM 4995	C	ASN	A	10	10.694	-4.319	6.813	1.00	5.70	A
25	ATOM 4996	O	ASN	A	10	9.636	-4.892	6.537	1.00	5.50	A

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	ATOM 4997	N	MET A	11	10.763	-3.054	7.208	1.00	6.01	A
	ATOM 4998	CA	MET A	11	9.597	-2.189	7.287	1.00	6.18	A
	ATOM 4999	CB	MET A	11	8.725	-2.548	8.500	1.00	9.09	A
	ATOM 5000	CG	MET A	11	9.416	-2.585	9.840	1.00	11.64	A
5	ATOM 5001	SD	MET A	11	8.242	-3.077	11.159	1.00	15.13	A
	ATOM 5002	CE	MET A	11	8.390	-4.861	11.133	1.00	14.75	A
	ATOM 5003	C	MET A	11	10.072	-0.749	7.378	1.00	5.10	A
	ATOM 5004	O	MET A	11	11.250	-0.502	7.633	1.00	4.65	A
	ATOM 5005	N	ARG A	12	9.168	0.193	7.132	1.00	4.17	A
10	ATOM 5006	CA	ARG A	12	9.518	1.607	7.220	1.00	3.48	A
	ATOM 5007	CB	ARG A	12	8.395	2.484	6.640	1.00	3.58	A
	ATOM 5008	CG	ARG A	12	8.129	2.254	5.147	1.00	4.20	A
	ATOM 5009	CD	ARG A	12	7.130	3.273	4.574	1.00	4.87	A
	ATOM 5010	NE	ARG A	12	5.888	3.302	5.344	1.00	5.23	A
15	ATOM 5011	CZ	ARG A	12	4.941	2.372	5.278	1.00	5.80	A
	ATOM 5012	NH1	ARG A	12	5.080	1.336	4.466	1.00	5.95	A
	ATOM 5013	NH2	ARG A	12	3.865	2.465	6.052	1.00	5.74	A
	ATOM 5014	C	ARG A	12	9.725	1.891	8.704	1.00	2.96	A
	ATOM 5015	O	ARG A	12	10.844	2.170	9.144	1.00	2.74	A
20	ATOM 5016	N	GLY A	13	8.639	1.808	9.466	1.00	2.56	A
	ATOM 5017	CA	GLY A	13	8.697	2.009	10.904	1.00	2.19	A
	ATOM 5018	C	GLY A	13	9.591	3.120	11.415	1.00	2.22	A
	ATOM 5019	O	GLY A	13	9.625	4.212	10.850	1.00	2.01	A
	ATOM 5020	N	ARG A	14	10.321	2.833	12.489	1.00	2.32	A
25	ATOM 5021	CA	ARG A	14	11.192	3.823	13.108	1.00	2.60	A

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	ATOM 5022	CB	ARG	A	14	11.457	3.436	14.570	1.00	2.99	A
	ATOM 5023	CG	ARG	A	14	10.223	3.584	15.442	1.00	4.04	A
	ATOM 5024	CD	ARG	A	14	10.492	3.265	16.906	1.00	5.12	A
	ATOM 5025	NE	ARG	A	14	9.320	3.584	17.718	1.00	6.44	A
5	ATOM 5026	CZ	ARG	A	14	8.960	4.815	18.073	1.00	7.09	A
	ATOM 5027	NH1	ARG	A	14	9.688	5.867	17.709	1.00	7.50	A
	ATOM 5028	NH2	ARG	A	14	7.841	4.998	18.765	1.00	7.96	A
	ATOM 5029	C	ARG	A	14	12.510	4.077	12.392	1.00	2.41	A
	ATOM 5030	O	ARG	A	14	13.238	4.997	12.750	1.00	2.83	A
10	ATOM 5031	N	ALA	A	15	12.822	3.277	11.378	1.00	2.21	A
	ATOM 5032	CA	ALA	A	15	14.068	3.484	10.648	1.00	1.80	A
	ATOM 5033	CB	ALA	A	15	14.627	2.144	10.156	1.00	2.27	A
	ATOM 5034	C	ALA	A	15	13.858	4.405	9.458	1.00	1.82	A
	ATOM 5035	O	ALA	A	15	14.815	4.976	8.938	1.00	1.57	A
15	ATOM 5036	N	GLU	A	16	12.610	4.575	9.033	1.00	1.93	A
	ATOM 5037	CA	GLU	A	16	12.359	5.372	7.840	1.00	1.94	A
	ATOM 5038	CB	GLU	A	16	10.870	5.346	7.482	1.00	2.14	A
	ATOM 5039	CG	GLU	A	16	10.579	5.687	6.016	1.00	2.49	A
	ATOM 5040	CD	GLU	A	16	11.126	4.665	5.011	1.00	3.04	A
20	ATOM 5041	OE1	GLU	A	16	11.667	3.615	5.422	1.00	3.42	A
	ATOM 5042	OE2	GLU	A	16	11.008	4.916	3.793	1.00	3.55	A
	ATOM 5043	C	GLU	A	16	12.875	6.801	7.878	1.00	1.89	A
	ATOM 5044	O	GLU	A	16	13.356	7.302	6.866	1.00	1.73	A
	ATOM 5045	N	ILE	A	17	12.807	7.460	9.030	1.00	1.19	A
25	ATOM 5046	CA	ILE	A	17	13.306	8.825	9.107	1.00	1.35	A

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	ATOM 5047	CB	ILE A	17	13.031	9.454	10.510	1.00	1.50	A
	ATOM 5048	CG2	ILE A	17	13.702	8.649	11.614	1.00	1.52	A
	ATOM 5049	CG1	ILE A	17	13.514	10.909	10.532	1.00	1.26	A
	ATOM 5050	CD1	ILE A	17	12.833	11.795	9.501	1.00	1.74	A
5	ATOM 5051	C	ILE A	17	14.807	8.856	8.760	1.00	1.44	A
	ATOM 5052	O	ILE A	17	15.275	9.775	8.079	1.00	2.26	A
	ATOM 5242	N	TRP A	39	16.279	-11.644	14.583	1.00	11.83	A
	ATOM 5243	CA	TRP A	39	16.330	-10.580	15.586	1.00	11.41	A
	ATOM 5244	CB	TRP A	39	14.938	-9.947	15.714	1.00	10.48	A
10	ATOM 5245	CG	TRP A	39	14.752	-8.981	16.856	1.00	9.62	A
	ATOM 5246	CD2	TRP A	39	15.630	-7.913	17.256	1.00	9.22	A
	ATOM 5247	CE2	TRP A	39	15.022	-7.269	18.356	1.00	9.06	A
	ATOM 5248	CE3	TRP A	39	16.865	-7.439	16.793	1.00	8.94	A
	ATOM 5249	CD1	TRP A	39	13.687	-8.935	17.705	1.00	9.52	A
15	ATOM 5250	NE1	TRP A	39	13.842	-7.915	18.607	1.00	9.30	A
	ATOM 5251	CZ2	TRP A	39	15.608	-6.173	19.005	1.00	8.71	A
	ATOM 5252	CZ3	TRP A	39	17.450	-6.345	17.442	1.00	8.93	A
	ATOM 5253	CH2	TRP A	39	16.817	-5.729	18.536	1.00	8.40	A
	ATOM 5254	C	TRP A	39	16.848	-11.032	16.960	1.00	11.66	A
20	ATOM 5255	O	TRP A	39	17.710	-10.382	17.547	1.00	11.72	A
	ATOM 5256	N	PRO A	40	16.337	-12.156	17.487	1.00	12.01	A
	ATOM 5257	CD	PRO A	40	15.261	-13.023	16.971	1.00	12.11	A
	ATOM 5258	CA	PRO A	40	16.795	-12.629	18.799	1.00	12.31	A
	ATOM 5259	CB	PRO A	40	16.171	-14.016	18.894	1.00	12.32	A
25	ATOM 5260	CG	PRO A	40	14.862	-13.816	18.203	1.00	12.38	A

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	ATOM 5261	C	PRO A	40	18.308	-12.656	19.023	1.00	12.59	A
	ATOM 5262	O	PRO A	40	18.799	-12.163	20.042	1.00	12.72	A
	ATOM 5263	N	GLU A	41	19.053	-13.223	18.081	1.00	12.84	A
	ATOM 5264	CA	GLU A	41	20.500	-13.309	18.231	1.00	13.09	A
5	ATOM 5265	CB	GLU A	41	21.054	-14.364	17.270	1.00	14.07	A
	ATOM 5266	CG	GLU A	41	20.459	-15.745	17.544	1.00	15.68	A
	ATOM 5267	CD	GLU A	41	20.995	-16.831	16.634	1.00	16.54	A
	ATOM 5268	OE1	GLU A	41	20.297	-17.854	16.473	1.00	17.39	A
	ATOM 5269	OE2	GLU A	41	22.109	-16.677	16.088	1.00	17.54	A
10	ATOM 5270	C	GLU A	41	21.229	-11.972	18.074	1.00	12.61	A
	ATOM 5271	O	GLU A	41	22.373	-11.827	18.506	1.00	12.75	A
	ATOM 5272	N	ILE A	42	20.566	-10.995	17.467	1.00	11.99	A
	ATOM 5273	CA	ILE A	42	21.160	-9.673	17.307	1.00	11.37	A
	ATOM 5274	CB	ILE A	42	20.596	-8.939	16.065	1.00	11.34	A
15	ATOM 5275	CG2	ILE A	42	20.978	-7.464	16.105	1.00	11.36	A
	ATOM 5276	CG1	ILE A	42	21.128	-9.596	14.788	1.00	11.71	A
	ATOM 5277	CD1	ILE A	42	20.546	-9.013	13.510	1.00	11.80	A
	ATOM 5278	C	ILE A	42	20.819	-8.870	18.561	1.00	11.10	A
	ATOM 5279	O	ILE A	42	21.665	-8.178	19.123	1.00	10.73	A
20	ATOM 5280	N	LYS A	43	19.571	-8.996	19.000	1.00	10.69	A
	ATOM 5281	CA	LYS A	43	19.075	-8.292	20.176	1.00	11.07	A
	ATOM 5282	CB	LYS A	43	17.665	-8.788	20.506	1.00	10.56	A
	ATOM 5283	CG	LYS A	43	17.027	-8.164	21.737	1.00	10.22	A
	ATOM 5284	CD	LYS A	43	15.654	-8.770	21.969	1.00	10.10	A
25	ATOM 5285	CE	LYS A	43	14.982	-8.200	23.204	1.00	9.67	A

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	ATOM 5286	NZ	LYS A	43	14.601	-6.767	23.037	1.00	9.62	A
	ATOM 5287	C	LYS A	43	19.986	-8.462	21.391	1.00	11.41	A
	ATOM 5288	O	LYS A	43	20.292	-7.495	22.089	1.00	11.31	A
	ATOM 5328	N	GLY A	49	18.949	-3.542	23.669	1.00	8.96	A
5	ATOM 5329	CA	GLY A	49	18.093	-4.495	22.982	1.00	8.21	A
	ATOM 5330	C	GLY A	49	16.991	-3.983	22.078	1.00	7.54	A
	ATOM 5331	O	GLY A	49	15.959	-4.642	21.937	1.00	7.64	A
	ATOM 5332	N	LYS A	50	17.203	-2.832	21.444	1.00	6.95	A
	ATOM 5333	CA	LYS A	50	16.197	-2.263	20.554	1.00	6.45	A
10	ATOM 5334	CB	LYS A	50	15.528	-1.042	21.199	1.00	7.37	A
	ATOM 5335	CG	LYS A	50	14.831	-1.283	22.528	1.00	9.43	A
	ATOM 5336	CD	LYS A	50	13.634	-2.197	22.385	1.00	10.69	A
	ATOM 5337	CE	LYS A	50	12.660	-2.004	23.550	1.00	11.86	A
	ATOM 5338	NZ	LYS A	50	13.354	-1.838	24.858	1.00	12.34	A
15	ATOM 5339	C	LYS A	50	16.803	-1.810	19.233	1.00	5.62	A
	ATOM 5340	O	LYS A	50	17.999	-1.515	19.152	1.00	4.99	A
	ATOM 5341	N	ILE A	51	15.968	-1.766	18.198	1.00	4.81	A
	ATOM 5342	CA	ILE A	51	16.386	-1.277	16.892	1.00	4.23	A
	ATOM 5343	CB	ILE A	51	16.427	-2.400	15.821	1.00	4.50	A
20	ATOM 5344	CG2	ILE A	51	17.736	-3.173	15.951	1.00	4.04	A
	ATOM 5345	CG1	ILE A	51	15.214	-3.320	15.954	1.00	4.67	A
	ATOM 5346	CD1	ILE A	51	15.125	-4.353	14.851	1.00	5.01	A
	ATOM 5347	C	ILE A	51	15.403	-0.173	16.503	1.00	3.91	A
	ATOM 5348	O	ILE A	51	14.295	-0.096	17.037	1.00	3.85	A
25	ATOM 5349	N	PRO A	52	15.769	0.677	15.540	1.00	3.47	A

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	ATOM 5350	CD	PRO A	52	14.929	1.849	15.221	1.00	3.53	A
	ATOM 5351	CA	PRO A	52	17.011	0.704	14.767	1.00	3.15	A
	ATOM 5352	CB	PRO A	52	16.712	1.735	13.687	1.00	3.26	A
	ATOM 5353	CG	PRO A	52	15.878	2.741	14.442	1.00	3.38	A
5	ATOM 5354	C	PRO A	52	18.294	1.063	15.490	1.00	3.11	A
	ATOM 5355	O	PRO A	52	18.288	1.690	16.547	1.00	3.03	A
	ATOM 5356	N	ILE A	53	19.394	0.632	14.887	1.00	3.27	A
	ATOM 5357	CA	ILE A	53	20.723	0.974	15.351	1.00	3.18	A
	ATOM 5358	CB	ILE A	53	21.495	-0.199	16.021	1.00	3.72	A
10	ATOM 5359	CG2	ILE A	53	20.858	-0.553	17.356	1.00	4.09	A
	ATOM 5360	CG1	ILE A	53	21.596	-1.386	15.064	1.00	4.16	A
	ATOM 5361	CD1	ILE A	53	22.466	-2.510	15.594	1.00	5.20	A
	ATOM 5362	C	ILE A	53	21.453	1.369	14.074	1.00	3.15	A
	ATOM 5363	O	ILE A	53	21.090	0.928	12.978	1.00	2.64	A
15	ATOM 5423	N	HIS A	62	22.206	4.210	18.799	1.00	3.50	A
	ATOM 5424	CA	HIS A	62	20.835	3.722	18.927	1.00	2.95	A
	ATOM 5425	CB	HIS A	62	20.705	2.722	20.090	1.00	3.26	A
	ATOM 5426	CG	HIS A	62	20.931	3.318	21.445	1.00	3.82	A
	ATOM 5427	CD2	HIS A	62	22.047	3.813	22.031	1.00	3.92	A
20	ATOM 5428	ND1	HIS A	62	19.923	3.438	22.376	1.00	4.07	A
	ATOM 5429	CE1	HIS A	62	20.406	3.984	23.478	1.00	3.93	A
	ATOM 5430	NE2	HIS A	62	21.692	4.222	23.295	1.00	4.38	A
	ATOM 5431	C	HIS A	62	19.890	4.910	19.100	1.00	2.81	A
	ATOM 5432	O	HIS A	62	20.342	6.050	19.215	1.00	2.85	A
25	ATOM 5433	N	GLN A	63	18.586	4.624	19.094	1.00	2.56	A

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	ATOM 5434	CA	GLN A	63	17.501	5.612	19.201	1.00	2.38	A
	ATOM 5435	CB	GLN A	63	17.730	6.586	20.366	1.00	2.32	A
	ATOM 5436	CG	GLN A	63	17.350	6.000	21.730	1.00	2.96	A
	ATOM 5437	CD	GLN A	63	15.851	5.823	21.898	1.00	3.14	A
5	ATOM 5438	OE1	GLN A	63	15.063	6.295	21.081	1.00	3.72	A
	ATOM 5439	NE2	GLN A	63	15.449	5.151	22.971	1.00	3.70	A
	ATOM 5440	C	GLN A	63	17.348	6.359	17.878	1.00	2.37	A
	ATOM 5441	O	GLN A	63	18.164	7.212	17.516	1.00	2.00	A
	ATOM 5442	N	SER A	64	16.279	6.028	17.160	1.00	2.43	A
10	ATOM 5443	CA	SER A	64	16.037	6.600	15.841	1.00	2.49	A
	ATOM 5444	CB	SER A	64	14.678	6.132	15.296	1.00	2.81	A
	ATOM 5445	OG	SER A	64	13.591	6.666	16.036	1.00	3.28	A
	ATOM 5446	C	SER A	64	16.138	8.113	15.705	1.00	2.23	A
	ATOM 5447	O	SER A	64	16.742	8.603	14.750	1.00	2.28	A
15	ATOM 5448	N	LEU A	65	15.553	8.854	16.639	1.00	2.47	A
	ATOM 5449	CA	LEU A	65	15.581	10.307	16.548	1.00	2.69	A
	ATOM 5450	CB	LEU A	65	14.465	10.899	17.409	1.00	3.06	A
	ATOM 5451	CG	LEU A	65	13.100	10.321	17.010	1.00	3.16	A
	ATOM 5452	CD1	LEU A	65	11.993	10.980	17.835	1.00	4.12	A
20	ATOM 5453	CD2	LEU A	65	12.854	10.538	15.522	1.00	3.74	A
	ATOM 5454	C	LEU A	65	16.935	10.886	16.925	1.00	2.92	A
	ATOM 5455	O	LEU A	65	17.330	11.935	16.411	1.00	3.32	A
	ATOM 5662	N	ASP A	93	9.345	15.416	18.542	1.00	3.67	A
	ATOM 5663	CA	ASP A	93	8.972	14.730	19.781	1.00	3.91	A
25	ATOM 5664	CB	ASP A	93	9.654	15.361	20.997	1.00	5.09	A

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	ATOM 5665	CG	ASP	A	93	11.041	14.797	21.243	1.00	6.18	A
	ATOM 5666	OD1	ASP	A	93	11.674	15.203	22.246	1.00	7.93	A
	ATOM 5667	OD2	ASP	A	93	11.495	13.945	20.442	1.00	7.01	A
	ATOM 5668	C	ASP	A	93	7.462	14.714	19.985	1.00	3.61	A
5	ATOM 5669	O	ASP	A	93	6.926	13.766	20.539	1.00	3.01	A
	ATOM 5670	N	THR	A	94	6.776	15.762	19.540	1.00	3.46	A
	ATOM 5671	CA	THR	A	94	5.325	15.808	19.676	1.00	3.57	A
	ATOM 5672	CB	THR	A	94	4.792	17.195	19.258	1.00	3.73	A
	ATOM 5673	OG1	THR	A	94	5.167	18.152	20.257	1.00	4.06	A
10	ATOM 5674	CG2	THR	A	94	3.273	17.186	19.101	1.00	3.88	A
	ATOM 5675	C	THR	A	94	4.721	14.702	18.811	1.00	3.74	A
	ATOM 5676	O	THR	A	94	3.789	14.001	19.223	1.00	3.84	A
	ATOM 5677	N	LEU	A	95	5.268	14.520	17.618	1.00	3.30	A
	ATOM 5678	CA	LEU	A	95	4.766	13.475	16.740	1.00	3.42	A
15	ATOM 5679	CB	LEU	A	95	5.377	13.609	15.346	1.00	3.94	A
	ATOM 5680	CG	LEU	A	95	4.919	14.812	14.518	1.00	4.38	A
	ATOM 5681	CD1	LEU	A	95	5.763	14.924	13.245	1.00	4.83	A
	ATOM 5682	CD2	LEU	A	95	3.444	14.650	14.184	1.00	5.05	A
	ATOM 5683	C	LEU	A	95	5.117	12.113	17.323	1.00	3.25	A
20	ATOM 5684	O	LEU	A	95	4.275	11.217	17.397	1.00	3.09	A
	ATOM 5685	N	ASP	A	96	6.364	11.960	17.756	1.00	3.25	A
	ATOM 5686	CA	ASP	A	96	6.796	10.687	18.305	1.00	3.69	A
	ATOM 5687	CB	ASP	A	96	8.301	10.702	18.585	1.00	4.27	A
	ATOM 5688	CG	ASP	A	96	8.891	9.305	18.644	1.00	4.99	A
25	ATOM 5689	OD1	ASP	A	96	8.774	8.574	17.637	1.00	6.02	A

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	ATOM 5690	OD2	ASP	A	96	9.478	8.933	19.684	1.00	6.06	A
	ATOM 5691	C	ASP	A	96	6.038	10.316	19.573	1.00	3.81	A
	ATOM 5692	O	ASP	A	96	5.791	9.137	19.819	1.00	3.60	A
	ATOM 5693	N	ASP	A	97	5.677	11.315	20.377	1.00	3.85	A
5	ATOM 5694	CA	ASP	A	97	4.924	11.062	21.608	1.00	4.32	A
	ATOM 5695	CB	ASP	A	97	4.600	12.377	22.332	1.00	5.15	A
	ATOM 5696	CG	ASP	A	97	5.754	12.898	23.172	1.00	5.96	A
	ATOM 5697	OD1	ASP	A	97	5.657	14.053	23.647	1.00	6.78	A
	ATOM 5698	OD2	ASP	A	97	6.748	12.163	23.377	1.00	6.61	A
10	ATOM 5699	C	ASP	A	97	3.614	10.355	21.261	1.00	4.57	A
	ATOM 5700	O	ASP	A	97	3.214	9.403	21.931	1.00	4.45	A
	ATOM 5701	N	PHE	A	98	2.947	10.823	20.210	1.00	4.32	A
	ATOM 5702	CA	PHE	A	98	1.680	10.219	19.809	1.00	4.70	A
	ATOM 5703	CB	PHE	A	98	0.956	11.086	18.778	1.00	5.18	A
15	ATOM 5704	CG	PHE	A	98	-0.415	10.574	18.423	1.00	5.70	A
	ATOM 5705	CD1	PHE	A	98	-1.420	10.518	19.385	1.00	6.58	A
	ATOM 5706	CD2	PHE	A	98	-0.690	10.107	17.144	1.00	6.14	A
	ATOM 5707	CE1	PHE	A	98	-2.681	10.001	19.077	1.00	6.93	A
	ATOM 5708	CE2	PHE	A	98	-1.950	9.587	16.825	1.00	6.50	A
20	ATOM 5709	CZ	PHE	A	98	-2.945	9.534	17.798	1.00	6.64	A
	ATOM 5710	C	PHE	A	98	1.876	8.825	19.232	1.00	4.66	A
	ATOM 5711	O	PHE	A	98	1.147	7.896	19.574	1.00	4.59	A
	ATOM 5712	N	MET	A	99	2.857	8.678	18.352	1.00	4.84	A
	ATOM 5713	CA	MET	A	99	3.117	7.377	17.749	1.00	5.40	A
25	ATOM 5714	CB	MET	A	99	4.299	7.464	16.777	1.00	5.46	A

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	ATOM 5715	CG	MET A	99	4.123	8.469	15.638	1.00	5.83	A
	ATOM 5716	SD	MET A	99	2.682	8.141	14.594	1.00	6.06	A
	ATOM 5717	CE	MET A	99	3.312	6.790	13.572	1.00	6.22	A
	ATOM 5718	C	MET A	99	3.420	6.339	18.832	1.00	6.00	A
5	ATOM 5719	O	MET A	99	2.994	5.188	18.739	1.00	6.05	A
	ATOM 5720	N	SER A	100	4.143	6.759	19.866	1.00	6.83	A
	ATOM 5721	CA	SER A	100	4.523	5.860	20.951	1.00	8.20	A
	ATOM 5722	CB	SER A	100	5.628	6.516	21.790	1.00	7.84	A
	ATOM 5723	OG	SER A	100	6.767	6.802	20.987	1.00	8.21	A
10	ATOM 5724	C	SER A	100	3.367	5.412	21.854	1.00	9.33	A
	ATOM 5725	O	SER A	100	3.524	4.476	22.646	1.00	9.63	A
	ATOM 5726	N	CYS A	101	2.211	6.062	21.721	1.00	10.45	A
	ATOM 5727	CA	CYS A	101	1.029	5.738	22.528	1.00	12.16	A
	ATOM 5728	CB	CYS A	101	-0.005	6.870	22.455	1.00	12.99	A
15	ATOM 5729	SG	CYS A	101	0.391	8.383	23.352	1.00	16.33	A
	ATOM 5730	C	CYS A	101	0.334	4.450	22.106	1.00	12.31	A
	ATOM 5731	O	CYS A	101	-0.382	3.836	22.900	1.00	12.62	A
	ATOM 5732	N	PHE A	102	0.526	4.044	20.857	1.00	12.65	A
	ATOM 5733	CA	PHE A	102	-0.137	2.843	20.368	1.00	13.00	A
20	ATOM 5734	CB	PHE A	102	-0.054	2.787	18.844	1.00	12.20	A
	ATOM 5735	CG	PHE A	102	-0.888	3.838	18.165	1.00	11.64	A
	ATOM 5736	CD1	PHE A	102	-0.514	5.179	18.211	1.00	11.24	A
	ATOM 5737	CD2	PHE A	102	-2.065	3.493	17.507	1.00	11.38	A
	ATOM 5738	CE1	PHE A	102	-1.297	6.164	17.610	1.00	11.11	A
25	ATOM 5739	CE2	PHE A	102	-2.858	4.468	16.902	1.00	11.06	A

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	ATOM 5740	CZ	PHE A 102	-2.474	5.809	16.953	1.00	10.93	A
	ATOM 5741	C	PHE A 102	0.382	1.557	20.998	1.00	13.83	A
	ATOM 5742	O	PHE A 102	1.580	1.275	20.975	1.00	13.59	A
	ATOM 5743	N	PRO A 103	-0.537	0.762	21.579	1.00	14.74	A
5	ATOM 5744	CD	PRO A 103	-1.976	1.093	21.609	1.00	14.92	A
	ATOM 5745	CA	PRO A 103	-0.297	-0.516	22.259	1.00	15.72	A
	ATOM 5746	CB	PRO A 103	-1.578	-0.707	23.061	1.00	15.57	A
	ATOM 5747	CG	PRO A 103	-2.608	-0.199	22.114	1.00	15.22	A
	ATOM 5748	C	PRO A 103	-0.008	-1.711	21.354	1.00	16.75	A
10	ATOM 5749	O	PRO A 103	-0.814	-2.639	21.265	1.00	16.71	A
	ATOM 5750	N	TRP A 104	1.146	-1.693	20.697	1.00	17.88	A
	ATOM 5751	CA	TRP A 104	1.527	-2.786	19.812	1.00	19.32	A
	ATOM 5752	CB	TRP A 104	2.792	-2.423	19.032	1.00	18.89	A
	ATOM 5753	CG	TRP A 104	2.548	-1.458	17.925	1.00	18.58	A
15	ATOM 5754	CD2	TRP A 104	2.010	-1.762	16.635	1.00	18.48	A
	ATOM 5755	CE2	TRP A 104	1.931	-0.548	15.918	1.00	18.52	A
	ATOM 5756	CE3	TRP A 104	1.584	-2.944	16.015	1.00	18.55	A
	ATOM 5757	CD1	TRP A 104	2.767	-0.110	17.942	1.00	18.43	A
	ATOM 5758	NE1	TRP A 104	2.400	0.444	16.739	1.00	18.43	A
20	ATOM 5759	CZ2	TRP A 104	1.443	-0.481	14.610	1.00	18.51	A
	ATOM 5760	CZ3	TRP A 104	1.099	-2.877	14.712	1.00	18.61	A
	ATOM 5761	CH2	TRP A 104	1.033	-1.651	14.026	1.00	18.57	A
	ATOM 5762	C	TRP A 104	1.756	-4.094	20.562	1.00	20.48	A
	ATOM 5763	O	TRP A 104	1.734	-5.170	19.964	1.00	20.69	A
25	ATOM 5764	N	ALA A 105	1.965	-4.000	21.870	1.00	21.92	A

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	ATOM 5765	CA	ALA A	105	2.214	-5.182	22.688	1.00	23.42	A
	ATOM 5766	CB	ALA A	105	3.036	-4.796	23.914	1.00	23.28	A
	ATOM 5767	C	ALA A	105	0.943	-5.910	23.120	1.00	24.45	A
	ATOM 5768	O	ALA A	105	1.013	-6.976	23.732	1.00	24.65	A
5	ATOM 5769	N	GLU A	106	-0.217	-5.342	22.802	1.00	25.65	A
	ATOM 5770	CA	GLU A	106	-1.485	-5.962	23.174	1.00	26.85	A
	ATOM 5771	CB	GLU A	106	-2.660	-5.132	22.655	1.00	27.04	A
	ATOM 5772	CG	GLU A	106	-4.013	-5.813	22.819	1.00	27.53	A
	ATOM 5773	CD	GLU A	106	-4.291	-6.224	24.252	1.00	27.76	A
10	ATOM 5774	OE1	GLU A	106	-4.226	-5.354	25.146	1.00	27.91	A
	ATOM 5775	OE2	GLU A	106	-4.580	-7.417	24.484	1.00	28.01	A
	ATOM 5776	C	GLU A	106	-1.599	-7.391	22.649	1.00	27.52	A
	ATOM 5777	O	GLU A	106	-1.223	-7.680	21.512	1.00	27.83	A
	ATOM 5778	N	LYS A	107	-2.130	-8.275	23.487	1.00	28.30	A
15	ATOM 5779	CA	LYS A	107	-2.300	-9.682	23.139	1.00	28.87	A
	ATOM 5780	CB	LYS A	107	-2.444	-10.514	24.414	1.00	29.16	A
	ATOM 5781	CG	LYS A	107	-1.271	-10.395	25.373	1.00	29.57	A
	ATOM 5782	CD	LYS A	107	0.009	-10.925	24.750	1.00	29.90	A
	ATOM 5783	CE	LYS A	107	1.156	-10.889	25.748	1.00	30.13	A
20	ATOM 5784	NZ	LYS A	107	0.857	-11.708	26.956	1.00	30.43	A
	ATOM 5785	C	LYS A	107	-3.509	-9.927	22.241	1.00	29.12	A
	ATOM 5786	O	LYS A	107	-3.376	-10.446	21.132	1.00	29.28	A
	ATOM 5787	N	LYS A	108	-4.689	-9.560	22.729	1.00	29.38	A
	ATOM 5788	CA	LYS A	108	-5.921	-9.745	21.972	1.00	29.63	A
25	ATOM 5789	CB	LYS A	108	-7.134	-9.496	22.872	1.00	30.00	A

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	ATOM 5790	CG	LYS A 108	-7.169	-10.367	24.123	1.00	30.56	A
	ATOM 5791	CD	LYS A 108	-8.456	-10.178	24.922	1.00	30.98	A
	ATOM 5792	CE	LYS A 108	-9.673	-10.768	24.211	1.00	31.33	A
	ATOM 5793	NZ	LYS A 108	-9.995	-10.085	22.924	1.00	31.67	A
5	ATOM 5794	C	LYS A 108	-5.969	-8.806	20.773	1.00	29.56	A
	ATOM 5795	O	LYS A 108	-6.053	-7.588	20.929	1.00	29.53	A
	ATOM 5796	N	GLN A 109	-5.912	-9.380	19.575	1.00	29.46	A
	ATOM 5797	CA	GLN A 109	-5.950	-8.594	18.348	1.00	29.31	A
	ATOM 5798	CB	GLN A 109	-5.908	-9.519	17.130	1.00	29.60	A
10	ATOM 5799	CG	GLN A 109	-5.886	-8.795	15.788	1.00	30.07	A
	ATOM 5800	CD	GLN A 109	-4.671	-7.898	15.624	1.00	30.20	A
	ATOM 5801	OE1	GLN A 109	-3.531	-8.347	15.745	1.00	30.51	A
	ATOM 5802	NE2	GLN A 109	-4.911	-6.623	15.341	1.00	30.44	A
	ATOM 5803	C	GLN A 109	-7.213	-7.740	18.306	1.00	29.07	A
15	ATOM 5804	O	GLN A 109	-7.197	-6.614	17.808	1.00	29.12	A
	ATOM 5805	N	ASP A 110	-8.304	-8.281	18.838	1.00	28.67	A
	ATOM 5806	CA	ASP A 110	-9.582	-7.576	18.871	1.00	28.20	A
	ATOM 5807	CB	ASP A 110	-10.662	-8.464	19.494	1.00	28.84	A
	ATOM 5808	CG	ASP A 110	-10.698	-9.855	18.892	1.00	29.35	A
20	ATOM 5809	OD1	ASP A 110	-11.510	-10.681	19.362	1.00	29.82	A
	ATOM 5810	OD2	ASP A 110	-9.918	-10.126	17.954	1.00	29.79	A
	ATOM 5811	C	ASP A 110	-9.450	-6.303	19.700	1.00	27.49	A
	ATOM 5812	O	ASP A 110	-9.794	-5.210	19.248	1.00	27.41	A
	ATOM 5813	N	VAL A 111	-8.952	-6.466	20.921	1.00	26.54	A
25	ATOM 5814	CA	VAL A 111	-8.765	-5.352	21.844	1.00	25.62	A

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	ATOM 5815	CB	VAL A 111	-8.261	-5.852	23.214	1.00	25.70	A
	ATOM 5816	CG1	VAL A 111	-8.118	-4.687	24.176	1.00	25.75	A
	ATOM 5817	CG2	VAL A 111	-9.220	-6.892	23.769	1.00	25.72	A
	ATOM 5818	C	VAL A 111	-7.751	-4.361	21.288	1.00	24.87	A
5	ATOM 5819	O	VAL A 111	-7.890	-3.150	21.457	1.00	24.76	A
	ATOM 5820	N	LYS A 112	-6.733	-4.893	20.623	1.00	23.93	A
	ATOM 5821	CA	LYS A 112	-5.679	-4.082	20.034	1.00	22.97	A
	ATOM 5822	CB	LYS A 112	-4.645	-4.995	19.376	1.00	23.32	A
	ATOM 5823	CG	LYS A 112	-3.397	-4.302	18.873	1.00	23.86	A
10	ATOM 5824	CD	LYS A 112	-2.432	-5.333	18.305	1.00	24.32	A
	ATOM 5825	CE	LYS A 112	-1.157	-4.697	17.788	1.00	24.73	A
	ATOM 5826	NZ	LYS A 112	-0.215	-5.733	17.271	1.00	25.05	A
	ATOM 5827	C	LYS A 112	-6.259	-3.114	19.007	1.00	22.11	A
	ATOM 5828	O	LYS A 112	-5.962	-1.920	19.031	1.00	21.79	A
15	ATOM 5829	N	GLU A 113	-7.092	-3.636	18.111	1.00	21.14	A
	ATOM 5830	CA	GLU A 113	-7.715	-2.815	17.079	1.00	20.14	A
	ATOM 5831	CB	GLU A 113	-8.529	-3.690	16.119	1.00	20.72	A
	ATOM 5832	CG	GLU A 113	-7.713	-4.763	15.412	1.00	21.85	A
	ATOM 5833	CD	GLU A 113	-8.491	-5.456	14.303	1.00	22.40	A
20	ATOM 5834	OE1	GLU A 113	-7.956	-6.422	13.717	1.00	22.88	A
	ATOM 5835	OE2	GLU A 113	-9.632	-5.032	14.010	1.00	23.04	A
	ATOM 5836	C	GLU A 113	-8.623	-1.766	17.712	1.00	19.20	A
	ATOM 5837	O	GLU A 113	-8.699	-0.632	17.240	1.00	18.59	A
	ATOM 5838	N	GLN A 114	-9.313	-2.157	18.780	1.00	18.24	A
25	ATOM 5839	CA	GLN A 114	-10.211	-1.252	19.492	1.00	17.58	A

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	ATOM 5840	CB	GLN A 114	-10.867	-1.989	20.665	1.00	18.40	A
	ATOM 5841	CG	GLN A 114	-11.701	-1.110	21.590	1.00	19.72	A
	ATOM 5842	CD	GLN A 114	-12.983	-0.617	20.951	1.00	20.35	A
	ATOM 5843	OE1	GLN A 114	-13.741	0.141	21.560	1.00	21.36	A
5	ATOM 5844	NE2	GLN A 114	-13.238	-1.045	19.721	1.00	21.11	A
	ATOM 5845	C	GLN A 114	-9.433	-0.044	20.011	1.00	16.47	A
	ATOM 5846	O	GLN A 114	-9.841	1.101	19.822	1.00	15.90	A
	ATOM 5847	N	MET A 115	-8.306	-0.308	20.664	1.00	15.39	A
	ATOM 5848	CA	MET A 115	-7.469	0.754	21.215	1.00	14.42	A
10	ATOM 5849	CB	MET A 115	-6.325	0.146	22.022	1.00	15.54	A
	ATOM 5850	CG	MET A 115	-6.800	-0.675	23.205	1.00	16.96	A
	ATOM 5851	SD	MET A 115	-5.448	-1.470	24.079	1.00	18.84	A
	ATOM 5852	CE	MET A 115	-5.262	-2.923	23.139	1.00	18.77	A
	ATOM 5853	C	MET A 115	-6.912	1.655	20.117	1.00	13.19	A
15	ATOM 5854	O	MET A 115	-6.872	2.877	20.267	1.00	12.74	A
	ATOM 5855	N	PHE A 116	-6.476	1.050	19.017	1.00	11.78	A
	ATOM 5856	CA	PHE A 116	-5.947	1.813	17.890	1.00	10.59	A
	ATOM 5857	CB	PHE A 116	-5.490	0.870	16.773	1.00	10.36	A
	ATOM 5858	CG	PHE A 116	-4.061	0.413	16.901	1.00	10.46	A
20	ATOM 5859	CD1	PHE A 116	-3.595	-0.162	18.081	1.00	10.57	A
	ATOM 5860	CD2	PHE A 116	-3.180	0.559	15.836	1.00	10.60	A
	ATOM 5861	CE1	PHE A 116	-2.264	-0.584	18.196	1.00	10.91	A
	ATOM 5862	CE2	PHE A 116	-1.850	0.140	15.940	1.00	10.80	A
	ATOM 5863	CZ	PHE A 116	-1.395	-0.431	17.123	1.00	10.66	A
25	ATOM 5864	C	PHE A 116	-7.028	2.746	17.352	1.00	9.91	A

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	ATOM 5865	O	PHE A 116	-6.784	3.926	17.107	1.00	9.44	A
	ATOM 6152	N	TYR A 152	9.540	13.762	9.073	1.00	2.77	A
	ATOM 6153	CA	TYR A 152	8.881	12.942	10.085	1.00	2.75	A
	ATOM 6154	CB	TYR A 152	9.375	13.285	11.493	1.00	2.46	A
5	ATOM 6155	CG	TYR A 152	9.275	12.107	12.439	1.00	2.52	A
	ATOM 6156	CD1	TYR A 152	9.745	10.850	12.057	1.00	2.65	A
	ATOM 6157	CE1	TYR A 152	9.704	9.767	12.931	1.00	2.76	A
	ATOM 6158	CD2	TYR A 152	8.749	12.251	13.727	1.00	2.68	A
	ATOM 6159	CE2	TYR A 152	8.700	11.166	14.614	1.00	2.62	A
10	ATOM 6160	CZ	TYR A 152	9.187	9.928	14.206	1.00	2.82	A
	ATOM 6161	OH	TYR A 152	9.200	8.848	15.069	1.00	3.50	A
	ATOM 6162	C	TYR A 152	7.367	13.051	10.016	1.00	2.91	A
	ATOM 6163	O	TYR A 152	6.660	12.070	10.255	1.00	2.96	A
	ATOM 6164	N	TRP A 153	6.863	14.237	9.696	1.00	3.18	A
15	ATOM 6165	CA	TRP A 153	5.424	14.392	9.562	1.00	3.43	A
	ATOM 6166	CB	TRP A 153	5.044	15.839	9.240	1.00	3.92	A
	ATOM 6167	CG	TRP A 153	3.631	15.957	8.702	1.00	4.79	A
	ATOM 6168	CD2	TRP A 153	2.425	15.511	9.340	1.00	5.21	A
	ATOM 6169	CE2	TRP A 153	1.359	15.767	8.446	1.00	5.55	A
20	ATOM 6170	CE3	TRP A 153	2.141	14.917	10.578	1.00	5.42	A
	ATOM 6171	CD1	TRP A 153	3.256	16.454	7.485	1.00	5.26	A
	ATOM 6172	NE1	TRP A 153	1.894	16.341	7.324	1.00	5.61	A
	ATOM 6173	CZ2	TRP A 153	0.029	15.449	8.749	1.00	5.49	A
	ATOM 6174	CZ3	TRP A 153	0.812	14.599	10.880	1.00	5.68	A
25	ATOM 6175	CH2	TRP A 153	-0.223	14.868	9.967	1.00	5.61	A

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	ATOM 6176	C	TRP A 153	4.929	13.497	8.428	1.00	3.45	A
	ATOM 6177	O	TRP A 153	3.935	12.797	8.576	1.00	3.37	A
	ATOM 6178	N	GLU A 154	5.618	13.518	7.291	1.00	3.56	A
	ATOM 6179	CA	GLU A 154	5.176	12.711	6.162	1.00	3.71	A
5	ATOM 6180	CB	GLU A 154	5.999	13.035	4.908	1.00	4.32	A
	ATOM 6181	CG	GLU A 154	5.412	12.438	3.622	1.00	5.29	A
	ATOM 6182	CD	GLU A 154	5.831	11.001	3.395	1.00	6.03	A
	ATOM 6183	OE1	GLU A 154	5.164	10.291	2.610	1.00	7.04	A
	ATOM 6184	OE2	GLU A 154	6.840	10.587	3.991	1.00	6.58	A
10	ATOM 6185	C	GLU A 154	5.242	11.218	6.467	1.00	3.29	A
	ATOM 6186	O	GLU A 154	4.349	10.463	6.092	1.00	3.50	A
	ATOM 6187	N	ILE A 155	6.290	10.801	7.166	1.00	3.02	A
	ATOM 6188	CA	ILE A 155	6.466	9.397	7.520	1.00	3.13	A
	ATOM 6189	CB	ILE A 155	7.888	9.182	8.105	1.00	2.70	A
15	ATOM 6190	CG2	ILE A 155	7.991	7.836	8.827	1.00	2.70	A
	ATOM 6191	CG1	ILE A 155	8.912	9.275	6.974	1.00	2.60	A
	ATOM 6192	CD1	ILE A 155	10.341	9.455	7.455	1.00	2.55	A
	ATOM 6193	C	ILE A 155	5.393	8.931	8.509	1.00	3.34	A
	ATOM 6194	O	ILE A 155	4.757	7.888	8.304	1.00	3.01	A
20	ATOM 6195	N	CYS A 156	5.178	9.708	9.570	1.00	3.50	A
	ATOM 6196	CA	CYS A 156	4.176	9.345	10.570	1.00	4.03	A
	ATOM 6197	CB	CYS A 156	4.227	10.298	11.771	1.00	4.29	A
	ATOM 6198	SG	CYS A 156	5.678	10.099	12.840	1.00	5.23	A
	ATOM 6199	C	CYS A 156	2.767	9.339	9.989	1.00	4.27	A
25	ATOM 6200	O	CYS A 156	2.009	8.390	10.199	1.00	4.23	A

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	ATOM 6201	N	SER A 157	2.419	10.391	9.254	1.00	4.32	A
	ATOM 6202	CA	SER A 157	1.085	10.469	8.668	1.00	4.75	A
	ATOM 6203	CB	SER A 157	0.838	11.865	8.072	1.00	5.10	A
	ATOM 6204	OG	SER A 157	1.761	12.194	7.047	1.00	5.43	A
5	ATOM 6205	C	SER A 157	0.852	9.369	7.631	1.00	4.95	A
	ATOM 6206	O	SER A 157	-0.264	8.874	7.487	1.00	4.57	A
	ATOM 6207	N	THR A 158	1.898	8.963	6.920	1.00	5.02	A
	ATOM 6208	CA	THR A 158	1.731	7.901	5.937	1.00	5.46	A
	ATOM 6209	CB	THR A 158	3.044	7.623	5.168	1.00	5.08	A
10	ATOM 6210	OG1	THR A 158	3.223	8.638	4.175	1.00	6.03	A
	ATOM 6211	CG2	THR A 158	3.002	6.255	4.484	1.00	5.35	A
	ATOM 6212	C	THR A 158	1.257	6.624	6.623	1.00	5.78	A
	ATOM 6213	O	THR A 158	0.330	5.963	6.153	1.00	6.22	A
	ATOM 6214	N	THR A 159	1.868	6.273	7.749	1.00	6.08	A
15	ATOM 6215	CA	THR A 159	1.439	5.056	8.416	1.00	6.86	A
	ATOM 6216	CB	THR A 159	2.511	4.534	9.380	1.00	7.60	A
	ATOM 6217	OG1	THR A 159	3.698	4.230	8.633	1.00	8.88	A
	ATOM 6218	CG2	THR A 159	2.029	3.261	10.065	1.00	8.45	A
	ATOM 6219	C	THR A 159	0.102	5.219	9.141	1.00	6.36	A
20	ATOM 6220	O	THR A 159	-0.716	4.304	9.136	1.00	6.28	A
	ATOM 6221	N	LEU A 160	-0.139	6.378	9.749	1.00	6.36	A
	ATOM 6222	CA	LEU A 160	-1.416	6.583	10.433	1.00	6.28	A
	ATOM 6223	CB	LEU A 160	-1.442	7.938	11.145	1.00	6.43	A
	ATOM 6224	CG	LEU A 160	-0.494	8.064	12.344	1.00	6.55	A
25	ATOM 6225	CD1	LEU A 160	-0.635	9.446	12.969	1.00	6.99	A

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	ATOM 6226	CD2	LEU A	160	-0.815	6.977	13.369	1.00	6.80	A
	ATOM 6227	C	LEU A	160	-2.567	6.505	9.428	1.00	6.52	A
	ATOM 6228	O	LEU A	160	-3.635	5.979	9.744	1.00	6.37	A
	ATOM 6229	N	LEU A	161	-2.344	7.026	8.224	1.00	6.39	A
5	ATOM 6230	CA	LEU A	161	-3.369	7.006	7.178	1.00	6.80	A
	ATOM 6231	CB	LEU A	161	-2.881	7.764	5.941	1.00	6.77	A
	ATOM 6232	CG	LEU A	161	-2.994	9.287	6.026	1.00	6.85	A
	ATOM 6233	CD1	LEU A	161	-2.211	9.934	4.893	1.00	6.96	A
	ATOM 6234	CD2	LEU A	161	-4.468	9.686	5.967	1.00	6.94	A
10	ATOM 6235	C	LEU A	161	-3.770	5.589	6.785	1.00	6.97	A
	ATOM 6236	O	LEU A	161	-4.869	5.370	6.272	1.00	7.11	A
	ATOM 6237	N	VAL A	162	-2.884	4.627	7.015	1.00	7.20	A
	ATOM 6238	CA	VAL A	162	-3.199	3.240	6.692	1.00	7.82	A
	ATOM 6239	CB	VAL A	162	-1.963	2.317	6.867	1.00	7.65	A
15	ATOM 6240	CG1	VAL A	162	-2.372	0.853	6.720	1.00	8.05	A
	ATOM 6241	CG2	VAL A	162	-0.905	2.673	5.830	1.00	7.94	A
	ATOM 6242	C	VAL A	162	-4.308	2.760	7.620	1.00	8.18	A
	ATOM 6243	O	VAL A	162	-5.197	2.014	7.205	1.00	8.53	A
	ATOM 6244	N	PHE A	163	-4.257	3.204	8.875	1.00	8.35	A
20	ATOM 6245	CA	PHE A	163	-5.251	2.813	9.871	1.00	8.79	A
	ATOM 6246	CB	PHE A	163	-4.612	2.753	11.263	1.00	9.22	A
	ATOM 6247	CG	PHE A	163	-3.511	1.746	11.376	1.00	10.12	A
	ATOM 6248	CD1	PHE A	163	-2.201	2.083	11.058	1.00	10.55	A
	ATOM 6249	CD2	PHE A	163	-3.792	0.440	11.773	1.00	10.59	A
25	ATOM 6250	CE1	PHE A	163	-1.186	1.129	11.135	1.00	10.94	A

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	ATOM 6251	CE2	PHE A 163	-2.787	-0.515	11.850	1.00	11.22	A
	ATOM 6252	CZ	PHE A 163	-1.481	-0.169	11.530	1.00	11.03	A
	ATOM 6253	C	PHE A 163	-6.454	3.745	9.920	1.00	8.73	A
	ATOM 6254	O	PHE A 163	-7.541	3.341	10.333	1.00	9.27	A
5	ATOM 6528	N	THR A 197	6.261	-2.354	2.065	1.00	5.54	A
	ATOM 6529	CA	THR A 197	5.873	-3.026	3.294	1.00	6.03	A
	ATOM 6530	CB	THR A 197	7.027	-2.988	4.330	1.00	6.06	A
	ATOM 6531	OG1	THR A 197	7.395	-1.626	4.585	1.00	6.14	A
	ATOM 6532	CG2	THR A 197	8.251	-3.733	3.796	1.00	6.10	A
10	ATOM 6533	C	THR A 197	4.634	-2.343	3.865	1.00	6.45	A
	ATOM 6534	O	THR A 197	4.355	-1.181	3.559	1.00	6.41	A
	ATOM 6535	N	LYS A 198	3.889	-3.065	4.691	1.00	7.24	A
	ATOM 6536	CA	LYS A 198	2.679	-2.512	5.272	1.00	7.84	A
	ATOM 6537	CB	LYS A 198	1.929	-3.596	6.046	1.00	8.50	A
15	ATOM 6538	CG	LYS A 198	0.529	-3.190	6.464	1.00	9.42	A
	ATOM 6539	CD	LYS A 198	-0.346	-3.015	5.237	1.00	10.37	A
	ATOM 6540	CE	LYS A 198	-1.794	-2.809	5.616	1.00	10.74	A
	ATOM 6541	NZ	LYS A 198	-2.644	-2.633	4.407	1.00	11.54	A
	ATOM 6542	C	LYS A 198	2.996	-1.350	6.203	1.00	7.94	A
20	ATOM 6543	O	LYS A 198	2.420	-0.263	6.082	1.00	8.01	A
	ATOM 6544	N	LEU A 199	3.929	-1.589	7.119	1.00	8.20	A
	ATOM 6545	CA	LEU A 199	4.335	-0.592	8.101	1.00	8.16	A
	ATOM 6546	CB	LEU A 199	4.199	-1.180	9.510	1.00	8.84	A
	ATOM 6547	CG	LEU A 199	2.859	-1.852	9.827	1.00	9.23	A
25	ATOM 6548	CD1	LEU A 199	2.923	-2.499	11.203	1.00	9.71	A

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	ATOM 6549	CD2 LEU A	199	1.739	-0.827	9.745	1.00	9.80	A
	ATOM 6550	C LEU A	199	5.775	-0.130	7.882	1.00	8.13	A
	ATOM 6551	OT1 LEU A	199	6.440	-0.652	6.959	1.00	7.55	A
	ATOM 6552	OT2 LEU A	199	6.216	0.753	8.649	1.00	8.21	A
5	ATOM 6613	N1 GSH H	4	12.088	5.233	20.820	1.00	7.13	H
	ATOM 6614	CA1 GSH H	4	12.962	4.197	20.254	1.00	7.03	H
	ATOM 6615	C1 GSH H	4	13.457	4.588	18.834	1.00	6.55	H
	ATOM 6616	O11 GSH H	4	12.879	5.504	18.242	1.00	6.42	H
	ATOM 6617	O12 GSH H	4	14.524	3.959	18.368	1.00	5.57	H
10	ATOM 6618	CB1 GSH H	4	12.145	2.885	20.215	1.00	7.92	H
	ATOM 6619	CG1 GSH H	4	13.006	1.603	20.044	1.00	8.47	H
	ATOM 6620	CD1 GSH H	4	12.022	0.396	19.925	1.00	9.25	H
	ATOM 6621	OE1 GSH H	4	11.170	0.182	20.803	1.00	9.64	H
	ATOM 6622	N2 GSH H	4	12.250	-0.419	18.881	1.00	9.52	H
15	ATOM 6623	CA2 GSH H	4	11.428	-1.623	18.662	1.00	10.30	H
	ATOM 6624	C2 GSH H	4	12.205	-2.870	19.063	1.00	10.93	H
	ATOM 6625	O2 GSH H	4	13.436	-2.897	19.121	1.00	9.41	H
	ATOM 6626	CB2 GSH H	4	11.161	-1.836	17.165	1.00	10.45	H
	ATOM 6627	SG2 GSH H	4	10.101	-0.583	16.421	1.00	11.44	H
20	ATOM 6628	N3 GSH H	4	11.453	-3.878	19.521	1.00	12.52	H
	ATOM 6629	CA3 GSH H	4	11.906	-5.282	19.488	1.00	13.88	H
	ATOM 6630	C3 GSH H	4	12.200	-5.722	20.899	1.00	14.49	H
	ATOM 6631	O31 GSH H	4	12.672	-6.865	21.036	1.00	15.15	H
	ATOM 6632	O32 GSH H	4	12.014	-4.897	21.826	1.00	15.40	H
25	ATOM 6675	MG+2 MG2 M	901	10.564	10.708	23.002	1.00	6.47	M

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	ATOM 6761	C1	HQL X	201	0.783	3.731	14.700	1.00	14.62	X
	ATOM 6762	C2	HQL X	201	1.692	4.118	15.845	1.00	14.59	X
	ATOM 6763	C3	HQL X	201	3.106	3.797	15.836	1.00	14.55	X
	ATOM 6764	C4	HQL X	201	3.711	3.097	14.685	1.00	14.90	X
5	ATOM 6765	C5	HQL X	201	5.187	2.827	14.734	1.00	15.13	X
	ATOM 6766	O1	HQL X	201	5.430	1.582	13.989	1.00	16.49	X
	ATOM 6767	C6	HQL X	201	6.385	0.713	14.568	1.00	18.14	X
	ATOM 6768	C7	HQL X	201	5.869	0.071	16.022	1.00	18.91	X
	ATOM 6769	C8	HQL X	201	5.795	-1.443	16.083	1.00	19.93	X
10	ATOM 6770	N1	HQL X	201	5.334	-2.091	14.799	1.00	20.61	X
	ATOM 6771	C9	HQL X	201	5.405	-3.554	15.187	1.00	21.81	X
	ATOM 6772	C10	HQL X	201	5.034	-4.554	14.080	1.00	23.26	X
	ATOM 6773	C11	HQL X	201	5.181	-5.967	14.572	1.00	24.56	X
	ATOM 6774	C12	HQL X	201	4.877	-6.836	13.391	1.00	25.39	X
15	ATOM 6775	N2	HQL X	201	3.772	-6.819	12.624	1.00	25.84	X
	ATOM 6776	N3	HQL X	201	3.922	-7.729	11.695	1.00	26.13	X
	ATOM 6777	N4	HQL X	201	5.093	-8.318	11.859	1.00	26.09	X
	ATOM 6778	N5	HQL X	201	5.695	-7.787	12.893	1.00	25.73	X
	ATOM 6779	C13	HQL X	201	6.228	-1.740	13.566	1.00	19.90	X
20	ATOM 6780	C14	HQL X	201	6.591	-0.245	13.299	1.00	18.75	X
	ATOM 6781	C15	HQL X	201	5.994	4.025	14.243	1.00	14.57	X
	ATOM 6782	C16	HQL X	201	6.642	4.886	15.312	1.00	14.43	X
	ATOM 6783	C17	HQL X	201	7.411	6.102	14.925	1.00	14.09	X
	ATOM 6784	C18	HQL X	201	7.560	6.480	13.475	1.00	14.22	X
25	ATOM 6785	C19	HQL X	201	6.931	5.623	12.396	1.00	14.18	X

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	ATOM 6786	C20	HQL	X	201	6.151	4.410	12.778	1.00	14.33	X
	ATOM 6787	C21	HQL	X	201	2.813	2.674	13.498	1.00	14.91	X
	ATOM 6788	C22	HQL	X	201	1.353	2.988	13.530	1.00	14.88	X
	ATOM 6790	OH2	WAT	S	2	14.771	8.489	19.484	1.00	5.47	S
5	ATOM 6791	OH2	WAT	S	3	11.680	1.507	3.580	1.00	5.07	S
	ATOM 6794	OH2	WAT	S	6	16.764	2.346	18.953	1.00	6.31	S
	ATOM 6797	OH2	WAT	S	9	10.902	6.761	11.193	1.00	3.72	S
	ATOM 6802	OH2	WAT	S	14	17.269	-1.249	7.632	1.00	5.08	S
	ATOM 6804	OH2	WAT	S	16	19.130	-0.458	21.382	1.00	6.03	S
10	ATOM 6807	OH2	WAT	S	19	9.886	-0.690	3.622	1.00	4.46	S
	ATOM 6809	OH2	WAT	S	21	11.248	7.004	14.090	1.00	4.99	S
	ATOM 6814	OH2	WAT	S	26	23.738	-1.909	12.157	1.00	5.26	S
	ATOM 6818	OH2	WAT	S	30	17.625	1.909	21.799	1.00	6.78	S
	ATOM 6824	OH2	WAT	S	36	16.161	2.164	24.178	1.00	8.59	S
15	ATOM 6825	OH2	WAT	S	37	6.016	5.686	6.917	1.00	8.02	S
	ATOM 6834	OH2	WAT	S	46	6.979	0.708	2.055	1.00	6.31	S
	ATOM 6838	OH2	WAT	S	50	12.098	8.108	20.192	1.00	7.43	S
	ATOM 6851	OH2	WAT	S	63	5.327	2.748	9.978	1.00	10.75	S
	ATOM 6862	OH2	WAT	S	74	7.157	4.594	9.351	1.00	8.69	S
20	ATOM 6875	OH2	WAT	S	87	13.436	2.712	24.346	1.00	11.43	S
	ATOM 6881	OH2	WAT	S	93	13.465	2.511	27.281	1.00	8.49	S
	ATOM 6917	OH2	WAT	S	129	4.790	-5.831	4.947	1.00	16.22	S
	ATOM 6923	OH2	WAT	S	135	11.522	-7.922	8.942	1.00	14.58	S
	ATOM 6927	OH2	WAT	S	139	7.332	5.571	25.452	1.00	13.15	S
25	ATOM 6931	OH2	WAT	S	144	4.347	8.725	24.399	1.00	18.59	S

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	ATOM 6936	OH2 WAT S	149	21.684	-0.730	22.365	1.00	19.24	S
	ATOM 6940	OH2 WAT S	153	6.829	6.961	4.592	1.00	11.46	S
	ATOM 6994	OH2 WAT S	207	9.472	5.801	21.506	1.00	15.51	S
	ATOM 6997	OH2 WAT S	210	5.042	-4.149	7.833	1.00	13.78	S
5	ATOM 7091	OH2 WAT S	304	3.700	2.599	19.458	1.00	18.38	S
	ATOM 7143	OH2 WAT S	356	4.462	6.079	25.441	1.00	21.81	S
	ATOM 7153	OH2 WAT S	366	14.674	-8.789	5.088	1.00	25.86	S
	ATOM 7162	OH2 WAT S	375	14.316	13.133	20.343	1.00	19.71	S
	ATOM 7174	OH2 WAT S	387	8.250	1.189	18.665	1.00	24.62	S
10	ATOM 7183	OH2 WAT S	396	20.328	-6.928	24.875	1.00	32.42	S
	ATOM 7223	OH2 WAT S	436	22.932	-6.039	12.661	1.00	30.30	S
	ATOM 7226	OH2 WAT S	439	10.226	-11.668	9.025	1.00	26.07	S
	ATOM 7227	OH2 WAT S	440	10.828	1.782	27.468	1.00	17.99	S
	ATOM 7231	OH2 WAT S	444	11.916	-14.217	16.326	1.00	26.35	S
15	ATOM 7244	OH2 WAT S	457	16.265	-1.371	28.167	1.00	34.60	S
	ATOM 7281	OH2 WAT S	494	7.021	-5.903	6.732	1.00	25.70	S
	ATOM 7290	OH2 WAT S	503	11.401	0.940	23.577	1.00	22.25	S
	ATOM 7313	OH2 WAT S	526	15.359	0.458	26.169	1.00	23.29	S
	ATOM 7325	OH2 WAT S	538	11.588	-8.884	22.349	1.00	25.83	S
20	ATOM 7341	OH2 WAT S	554	10.740	-8.906	19.123	1.00	36.43	S
	ATOM 7365	OH2 WAT S	578	9.748	-2.511	21.886	1.00	32.74	S
	ATOM 7428	OH2 WAT S	641	9.454	12.503	23.240	1.00	7.54	S
	ATOM 7429	OH2 WAT S	642	9.887	9.966	24.786	1.00	10.81	S
	ATOM 7430	OH2 WAT S	643	12.091	11.779	23.976	1.00	13.97	S
25	ATOM 7431	OH2 WAT S	644	11.037	11.297	21.097	1.00	12.32	S

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	ATOM 7432	OH2 WAT S	645	8.928	9.669	22.178	1.00	9.54	S
	ATOM 7433	OH2 WAT S	646	11.790	9.079	22.827	1.00	8.22	S
	ATOM 7445	OH2 WAT S	658	8.377	3.747	23.391	1.00	28.44	S
	ATOM 7448	OH2 WAT S	661	10.331	-0.751	28.752	1.00	36.87	S
5	ATOM 7449	OH2 WAT S	662	11.270	-5.110	29.771	1.00	27.40	S
	ATOM 7473	OH2 WAT S	686	6.297	-7.443	3.798	1.00	34.15	S
	ATOM 7482	OH2 WAT S	695	2.766	-7.409	6.323	1.00	31.70	S
	ATOM 7483	OH2 WAT S	696	3.236	-5.622	9.446	1.00	30.92	S
	ATOM 7490	OH2 WAT S	703	7.547	8.295	24.274	1.00	13.98	S
10	ATOM 7498	OH2 WAT S	711	23.720	0.535	21.093	1.00	33.19	S
	ATOM 7518	OH2 WAT S	731	11.607	-11.967	17.559	1.00	29.38	S
	ATOM 7606	OH2 WAT S	819	13.230	-5.747	25.483	1.00	31.58	S
	ATOM 7607	OH2 WAT S	820	15.415	-8.549	26.956	1.00	34.91	S
	ATOM 7646	OH2 WAT S	859	19.195	-6.110	26.916	1.00	43.51	S
15	ATOM 7663	OH2 WAT S	876	9.450	-8.128	10.745	1.00	28.17	S
	ATOM 7664	OH2 WAT S	877	6.964	-8.045	9.036	1.00	32.76	S
	ATOM 7677	OH2 WAT S	890	-4.103	-2.947	14.907	1.00	31.94	S
	ATOM 7685	OH2 WAT S	898	0.382	-6.331	13.311	1.00	40.22	S
	ATOM 7703	OH2 WAT S	916	12.503	-10.886	20.792	1.00	32.79	S
20	ATOM 7726	OH2 WAT S	939	9.361	1.904	25.025	1.00	24.74	S
	ATOM 7733	OH2 WAT S	946	6.220	10.170	25.032	1.00	33.80	S
	ATOM 7801	OH2 WAT S	1014	9.686	-9.232	5.261	1.00	31.69	S
	ATOM 7802	OH2 WAT S	1015	3.009	-1.511	23.142	1.00	36.99	S
	ATOM 7825	OH2 WAT S	1038	12.443	-8.837	27.155	1.00	37.43	S
25	ATOM 7836	OH2 WAT S	1049	2.595	0.473	29.257	1.00	34.46	S

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	ATOM 7879	OH2 WAT S1092	8.471	-3.139	15.245	1.00	24.42	S
	ATOM 7889	OH2 WAT S1102	8.537	-5.669	15.531	1.00	33.36	S
	ATOM 7890	OH2 WAT S1103	9.120	-7.616	16.968	1.00	37.15	S
	ATOM 7932	OH2 WAT S1147	2.722	0.246	25.232	1.00	38.87	S
5	ATOM 7933	OH2 WAT S1148	1.715	2.322	24.218	1.00	34.69	S
	ATOM 7946	OH2 WAT S1161	12.929	-1.852	29.410	1.00	40.70	S
	ATOM 8049	OH2 WAT S1264	5.506	-4.229	21.028	1.00	36.38	S
	ATOM 8050	OH2 WAT S1265	7.355	-0.482	24.373	1.00	39.74	S
	ATOM 8051	OH2 WAT S1266	5.564	-1.958	27.066	1.00	38.45	S
10	ATOM 8054	OH2 WAT S1269	1.047	-2.647	28.146	1.00	39.12	S

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SEQUENCE LISTING

<110> Japan Science and Technology Agency

<110> Osaka Bioscience Institute

<110> RIKEN

<120> Three-Dimensional Structure Of Prostaglandin D Synthase and
Utilization Thereof

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<151> 2001-11-12

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30

Ile Glu Gln Ala Asp Trp Pro Glu Ile Lys Ser Thr Leu Pro Phe Gly

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Ala Ile Ala Arg Tyr Leu Thr Lys Asn Thr Asp Leu Ala Gly Asn Thr

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Gln Met Phe Asn Glu Leu Leu Thr Tyr Asn Ala Pro His Leu Met Gln

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Val Phe Lys Pro Asp Leu Leu Asp Asn His Pro Arg Leu Val Thr Leu

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Arg Lys Lys Val Gln Ala Ile Pro Ala Val Ala Asn Trp Ile Lys Arg

180185190

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Arg Pro Gln Thr Lys Leu

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WHAT IS CLAIMED IS:

1. A complex of human calcium-type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1 and glutathione which has three dimensional structure represented by the structural coordinates in Table 1.
5
2. A complex of human magnesium-type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1 and glutathione which has three dimensional structure represented by the structural coordinates in Table 2.
- 10 3. A complex of human calcium-type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1, glutathione and 9,11-dideoxy -9 α ,11 α methanoepoxyprostaglandin F_2 , which has three dimensional structure represented by the structural coordinates in
15 Table 3.
4. A complex of human magnesium-type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1, glutathione and 9,11-dideoxy -9 α ,11 α - methanoepoxyprostaglandin F_2 , which has three dimensional
20 structure represented by structural coordinate in Table 4.
5. A complex of human calcium-type hematopoietic PGDS having amino acid sequence of SEQ. ID NO 1, glutathione and 9,11-dideoxy -9 α ,11 α - epoxymetanoprostaglandin F_2 , which has three dimensional
25 structure represented by the structural coordinates in

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Table 5.

6. A complex of human magnesium-type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1, glutathione and 9,11-dideoxy -9 α ,11 α -
5 epoxymetanoprostaglandin F₂, which has three dimensional structure represented by the structural coordinates in Table 6.

7. A complex of human calcium-type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1,
10 glutathione and 1-amino-4-{4-[4-chloro-6-(2-sulfo-phenylamino)-[1,3,5]triazine-2-ylmethyl]-3-sulfo-phenylamino}-9,10-dioxo-9,10-dihydro-anthracene-2-sulfonic acid which has three dimensional structure represented by the structural coordinates in Table 7.

15 8. A complex of human magnesium type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1, glutathione and 4-benzhydryloxy-1-{3-(1H-tetrazol-5-yl)-propyl}piperidine which has three dimensional structure represented by the structural coordinates in Table 8.

20 9. Structural coordinates represented in Table 1 of a complex of human calcium-type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1 and glutathione.

10. Structural coordinates represented in Table 2 of a complex of human magnesium-type hematopoietic PGDS having
25 an amino acid sequence of SEQ. ID NO 1 and glutathione.

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11. Structural coordinates represented in Table 3 of a complex of human calcium-type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1, glutathione and 9,11-dideoxy -9 α ,11 α -methanoepoxyprostaglandin F_{2 α} .

5 12. Structural coordinates represented in Table 4 of a complex of human magnesium-type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1, glutathione and 9,11-dideoxy -9 α ,11 α -methanoepoxyprostaglandin F_{2 α} .

10 13. Structural coordinates represented in Table 5 of a complex of human calcium-type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1, glutathione and 9,11-dideoxy -9 α ,11 α -epoxymetanoprostaglandin F_{2 α} .

15 14. Structural coordinates represented in Table 6 of a complex of human magnesium-type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1, glutathione and 9,11-dideoxy -9 α ,11 α -epoxymetanoprostaglandin F_{2 α} .

20 15. Structural coordinates represented in Table 7 of a complex of human calcium-type hematopoietic PGDS having an amino acid sequence of SEQ. ID NO 1, glutathione and 1-amino-4-(4-[4-chloro-6-(2-sulfo-phenylamino)-[1,3,5]triazine-2-ylmethyl]-3-sulfo-phenylamino)-9,10-dioxo-9,10-dihydro-anthracene-2-sulfonic acid.

25 16. Structural coordinates represented in Table 8 of a complex of human magnesium type hematopoietic PGDS having amino acid sequence of SEQ. ID NO 1, glutathione and 4-

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benzhydryloxy-1-(3-(1H-tetrazol-5-yl)-propyl)piperidine.

17. Use of at least one structural coordinates
selected from the group of structural coordinates
represented by Tables 1 to 8 for selection of a compound
5 inhibiting human hematopoietic PGDS.

18. A method for selecting an inhibitor of human
hematopoietic PGDS, comprising steps of:

(a) providing at least one structural coordinate
selected from the group consisting of structural
10 coordinates represented in Table 1-8 which characterizes an
active site of human hematopoietic PGDS;

(b) providing steric structure of a candidate
compound; and

(c) fitting the candidate to the active site of human
15 hematopoietic PGDS to select the inhibitor.

19. A method in accordance with Claim 18 which
further comprising:

(d) contacting the selected compound with the enzyme
in the presence of prostaglandin H₂ to confirm an ability
20 of the compound to inhibit the enzymatic activity of PGDS.

20. A method in accordance with Claim 18 or 19 which
further comprising measuring whether the inhibitor has at
least one biological activity selected the group consisting
of anti-allergic activity, sleep control activity, anti-
25 obesity activity and brain wound healing activity.

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21. An inhibitor of human hematopoietic PGDS selected by the method of Claim 18 or 19.

22. An anti-allergic agent, a sleep control agent, an anti-obestic agent or a brain wound healing agent selected
5 by the method of Claim 20.

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Application number / numéro de demande: JP02/09994Figures: all (1 to 6)

Pages: _____

Unscannable items
received with this application.

(Request original documents in File Prep. Section on the 10th floor)

Documents reçu avec cette demande ne pouvant être balayés
(Commander les documents originaux dans la section de préparation des dossiers au
10^{ème} étage)